7,7-Dimethyl-2'-*N*-phenylhydrazine-bicyclo[2.2.1]heptane-1-carboxylic acid (2)

To a solution of ketopinic acid **1** (20.00 g, 109.80 mmole) and phenylhydrazine (14.20 g, 131.3 mmole) in CH_2Cl_2 (545 mL) was added acetic acid (1.30 g, 21.65 mmole) dropwise at room temperature. This was allowed to stir for 5 h, and the volume was concentrated to about 50 mL and hexane was added until solid precipitate. The precipitate was collected and crystallized from ethyl acetate to give 28.3 g (95%) of **2** as a colorless crystal. ^{1}H NMR ($CDCl_3$, 200 MHz) δ 7.33-7.25 (m, 2H), 7.00-6.89 (m, 3H), 2.65-2.46 (m, 2H), 2.16-2.08 (m, 3H), 1.85 (ddd, 1H, J=12.4, 9.4, 4.0 Hz), 1.45-1.28 (m, 1H), 1.30 (s, 3H), 0.92 (s, 3H); ^{13}C NMR ($CDCl_3$, 50 MHz) δ 172.45, 157.46, 144,06, 129.56, 121.11, 113.05, 59.93, 51.83, 44.50, 32.82, 32.36, 28.16, 19.97, 19.95; HRMS *m/z* 272.1487 (calcd for $C_{16}H_{20}N_2O_2$: 272.1525). Anal. calcd for $C_{16}H_{20}N_2O_2$: C 70.56; H 7.40. Found: C 70.32; H 7.54.

7,7-Dimethyl-2'-phenyl-2',4'-dihydro-pyrazol-3'-one-bicyclo[2.2.1]heptane (3)

To a solution of **2** (9.00 g, 33.07 mmole) in ethyl acetate (660 mL) was added Et_3N (3.40 g, 33.60 mmole) at room temperature. This was followed by the addition of $SOCl_2$ (3.10 mL, 42.52 mmole) dropwise and the resulting mixture was brought to 60 °C for 5 h and quenched with H_2O. The products were extracted with ethyl acetate and the layers were separated. The organic layer washed with brine and dried over Na_2SO_4. The solvent was removed *in vacuo* and the product purified by flash column chromatography, using hexane/ethyl acetate (10:1) as eluent, to give 8.40 g (99%) of **3** as a white solid. ^{1}H NMR ($CDCl_3$, 200 MHz) δ 7.93-7.87 (m, 2H), 7.42-7.34 (m, 2H), 7.19-7.11 (m, 1H), 2.71 (dt, 1H, J=17.8, 3.3 Hz), 2.43-2.33 (m, 2H), 2.31-2.17 (m, 2H), 1.81 (ddd, 1H, J=12.0, 9.3, 3.6 Hz), 1.56 (ddd, 1H, J=11.6, 9.3, 3.6 Hz), 1.26 (s, 3H), 1.00 (s, 3H); ^{13}C NMR ($CDCl_3$, 50 MHz) δ 173.21, 170.92, 137.42, 127.12, 122.90, 116.96, 63.43, 48.61, 47.60, 30.26, 25.35, 24.10, 17.43, 16.85; HRMS *m/z* 254.1412 (calcd for $C_{16}H_{18}NO_2$: 254.1419).

7,7-Dimethyl-2'-phenyl-pyrazol-3'-one-bicyclo[2.2.1]heptane (4)

To a solution of **3** (4.00 g, 15.74 mmole) in MeOH (78 mL) was added $NaBH_4$ (6.0 g, 158.60 mmole) over a course of 1 h at room temperature. The solvent was partial removed by rotovapor and the mixture was added CH_2Cl_2/H_2O. The layers were separated and the organic layer washed with brine and dried over Na_2SO_4. The solvent was removed *in vacuo*, and the product purified by flash column chromatography, using hexane/ethyl acetate (10:1) as eluent, to give 3.80 g (94%) of **4** as a white solid. ^{1}H NMR ($CDCl_3$, 200 MHz) δ 7.81-7.75 (m, 2H), 7.38-7.33 (m, 2H), 7.14-7.06 (m, 1H), 4.40 (br., 1H), 3.71 (dd, 1H, J=8.2, 4.6 Hz), 2.30-2.18 (m, 2H), 2.06-1.86 (m, 2H), 1.82 (dd, 1H, J=13.1, 8.3 Hz), 1.55-1.29 (m, 2H), 1.25 (s, 3H), 1.11 (s, 3H); ^{13}C NMR ($CDCl_3$, 50 MHz) δ 170.54, 138.87, 128.71, 124.23, 118.59, 64.32, 59.84, 51.81, 46.85, 36.58, 28.65, 26.69, 20.82, 20.27; HRMS *m/z* 256.1584 (calcd for $C_{16}H_{20}N_2O$: 256.1576). Anal. calcd for $C_{16}H_{20}N_2O$: C 74.97; H 7.86. Found: C 75.20; H 7.88.

***N*-Acryloyl acrylate (5)**

To a solution of **4** (4.00 g, 15.55 mmole) in CH_2Cl_2 (155 mL) was added Et_3N (3.2 mL, 23.33 mmole) at 0 °C under N_2 atmosphere. This was followed by the addition of acryloyl chloride (1.54 mL, 18.66 mmole) dropwise and the mixture was stirred for 30 min. The mixture was quenched with H_2O (15 mL)

and extracted with CH_2Cl_2 (50 mL x 2). The layers were separated and the organic layer washed with brine and dried over Na_2SO_4. The solvent was removed *in vacuo*, and the product crystallized from hexane/ethyl acetate (6:1) to give 4.66 g (96%) of **5** as a colorless crystal. ^{1}H NMR ($CDCl_3$, 200 MHz) δ 7.39-7.29 (m, 4H), 7.18-7.12 (m, 1H), 6.38 (dd, 1H, J=16.8, 2.6 Hz), 6.25 (dd, 1H, J=16.8, 9.4 Hz), 5.68 (dd, 1H, J=9.4, 2.6 Hz), 4.15 (dd, 1H, J=7.8, 5.0 Hz), 2.75-2.65 (m, 1H), 2.36-2.24 (m, 1H), 2.16-2.06 (m, 1H), 2.03-1.95 (m, 2H), 1.48-1.26 (m, 2H), 1.14 (s, 3H), 1.11 (s, 3H); ^{13}C NMR ($CDCl_3$, 50 MHz) δ 170.60, 164.57, 138.78, 129.77, 128.54, 127.57, 125.63, 121.14, 66.73, 59.10, 53.18, 46.46, 38.66, 28.24, 26.72, 20.15, 20.01. HRMS *m/z* 310.1682 (calcd for $C_{19}H_{22}N_2O_2$: 310.1681).

General procedure for the preparation of 6

To a solution of **5** (0.10 g, 0.32 mmole) in DMSO (1.6 mL) was added excess acetaldehyde (0.15 g, 10 equiv) dropwise and DABCO (4 mg, 0.1 equiv) at room temperature under N_2 atmosphere. The resulting mixture was allowed to stir for 48 h and quenched with EtOAc/H_2O (30 mL, 2/1). The layers were separated and the organic layer washed with brine and dried over Na_2SO_4. The solvent was removed *in vacuo*, and the product purified by flash column chromatography, using hexane/ethyl acetate (2:1) as eluent, to give 95 mg (88%) of **6a** as a white solid. ^{1}H NMR ($CDCl_3$, 200 MHz) δ 7.41-7.25 (m, 3H), 7.36-7.14 (m, 2H), 5.75 (d, 1H, J=1.2 Hz), 5.66 (s, 1H), 4.54 (q, 1H, J=6.6 Hz), 4.31 (dd, 1H, J=8.0, 5.1 Hz), 2.50-2.39 (m, 1H), 2.38-2.23 (m, 1H), 2.08-1.85 (m, 4H), 1.48-1.32 (m, 1H), 1.39 (d, 3H, J=6.6 Hz), 1.17 (s, 3H), 1.15 (s, 3H); ^{13}C NMR ($CDCl_3$, 50 MHz) δ 169.85, 167.33, 146.91, 137.95, 128.72, 125.98, 121.09, 119.68, 69.61, 67.51, 59.29, 52.03, 47.01, 39.93, 28.66, 26.51, 21.88, 20.51, 19.82; HRMS *m/z* 354.1960 (calcd for $C_{21}H_{26}N_2O_3$: 354.1943).

6b: ^{1}H NMR ($CDCl_3$, 200 MHz) δ 7.40–7.26 (m, 3H), 7.21–7.13 (m, 2H), 5.68 (d, 1H, J=1.0 Hz), 5.66 (s, 1H), 4.30 (dd, 1H, J=7.6, 5.2 Hz), 4.21 (t, 1H, J=6.8 Hz), 2.55-2.43 (m, 1H), 2.35-2.22 (m, 1H), 2.05-1.84 (m, 3H), 1.76-1.63 (m, 2H), 1.48-1.25 (m, 3H), 1.16 (s, 3H), 1.14 (s, 3H), 0.95 (t, 3H, J=7.2 Hz); ^{13}C NMR ($CDCl_3$, 50 MHz) δ 169.90, 167.08, 146.05, 137.95, 128.66, 125.92, 121.09, 120.17, 73.56, 69.63, 59.28, 51.97, 46.99, 39.92, 29.18, 28.65, 26.48, 20.48, 19.77, 10.26; HRMS *m/z* 368.2127 (calcd for $C_{22}H_{28}N_2O_3$: 368.2100).). Anal. calcd for $C_{22}H_{28}N_2O_3$: C 71.71; H 7.66; N 7.60 Found: C 71.76; H 7.41; N 7.43.

6c: ^{1}H NMR ($CDCl_3$, 200 MHz) δ 7.41-7.14 (m, 10H), 5.68 (d, 1H, J=1.0 Hz), 5.66 (s, 1H), 4.35-4.25 (m, 2H), 2.83-2.74 (m, 1H), 2.70-2.58 (m, 1H), 2.53-2.43 (m, 1H), 2.35-2.26 (m, 1H), 2.07-1.86 (m, 6H), 1.49-1.28 (m, 2H), 1.15 (s, 3H), 1.14 (s, 3H); ^{13}C NMR ($CDCl_3$, 50 MHz) δ 169.88, 166.91, 146.31, 141.47, 137.95, 128.69, 128.49, 128.45, 125.96, 121.11, 120.21, 71.31, 69.64, 59.29, 51.97, 46.99, 39.86, 37.98, 32.03, 28.63, 26.48, 20.48, 19.77; HRMS *m/z* 444.2402 (calcd for $C_{28}H_{32}N_2O_3$: 444.2413). Anal. calcd for $C_{28}H_{32}N_2O_3$: C 75.65; H 7.26; N 6.30. Found: C 75.38; H 7.27; N 6.17.

6d: ^{1}H NMR ($CDCl_3$, 200 MHz) δ 7.39-7.19 (m, 3H), 7.18-7.13 (m, 2H), 5.69 (s, 1H), 5.62 (s, 1H), 4.39 (dd, 1H, J=9.6, 3.6 Hz), 4.29 (dd, 1H, J=8.0, 5.2 Hz), 2.85 (s, br. 1H), 2.51-2.40 (m, 1H), 2.29-2.03 (m, 1H), 2.01-1.67 (m, 4H), 1.65-1.56 (m, 1H), 1.41-1.26 (m, 3H), 1.15 (s, 3H), 1.12 (s, 3H), 0.90 (d, 3H, J=3.8 Hz), 0.87 (d, 3H, J=3.8 Hz); ^{13}C NMR ($CDCl_3$, 50 MHz) δ 169.85, 166.94, 146.88,

137.84, 128.42, 125.61, 120.86, 119.65, 69.61, 69.29, 59.08, 51.81, 46.78, 45.29, 39.66, 28.40, 26.28, 24.25, 23.18, 21.20, 20.32, 19.60.

6e: ^{1}H NMR ($CDCl_3$, 200 MHz) δ 7.39-7.26 (m, 8H), 7.25-7.14 (m, 2H), 5.75 (d, 1H, J=1.0 Hz), 5.69 (s, 1H), 5.58 (s, 1H), 3.85 (dd, 1H, J=8.0, 5.2 Hz), 3.40 (s, br. 1H), 2.24-2.13 (m, 1H), 2.12-1.90 (m, 1H), 1.77-1.61 (m, 2H), 1.25-1.13 (m, 3H), 1.04 (s, 3H), 0.85 (s, 3H); ^{13}C NMR ($CDCl_3$, 50 MHz) δ 169.75, 168.06, 145.72, 140.62, 138.02, 128.71, 128.57, 128.19, 126.84, 125.81, 120.98, 120.80, 73.97, 68.63, 58.99, 52.32, 46.69, 39.97, 28.51, 26.46, 20.32, 19.68; HRMS *m/z* 416.2138 (calcd for $C_{26}H_{28}N_2O_3$: 416.2100).

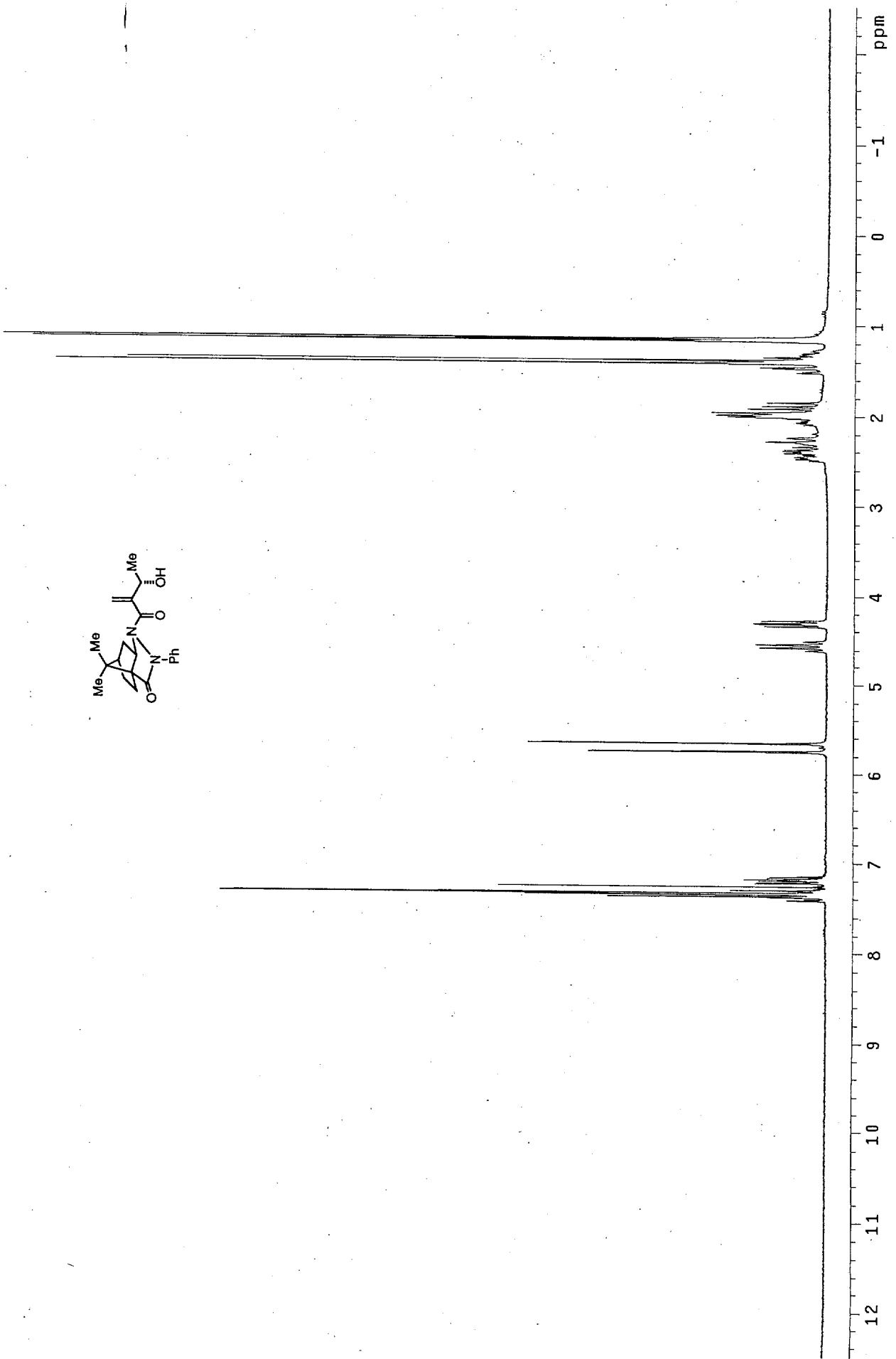
General procedure for the preparation of 7

To a solution of **5** (0.10 g, 0.32 mmole) in THF/H_2O (3.2 mL, 5/1) was added excess acetaldehyde (0.15 g, 10 equiv) dropwise and DABCO (8 mg, 0.2 equiv) at room temperature under N_2 atmosphere. The resulting mixture was allowed to stir for 48 h and quenched with EtOAc/ H_2O (30 mL, 2/1). The layers were separated and the organic layer washed with brine and dried over Na_2SO_4. The solvent was removed *in vacuo*, and the product purified by flash column chromatography, using hexane/ethyl acetate (2:1) as eluent, to give 83 mg (73%) of **7a** as a white solid. ^{1}H NMR ($CDCl_3$, 200 MHz) δ 7.41-7.22 (m, 3H), 7.21-7.15 (m, 2H), 5.69 (d, 1H, J=1.4 Hz), 5.65 (s, 1H), 4.57 (q, 1H, J=6.4 Hz), 4.32 (dd, 1H, J=7.6, 5.2 Hz), 2.59-2.51 (m, 1H), 2.48-2.23 (m, 1H), 2.06-1.83 (m, 4H), 1.46-1.25 (m, 1H), 1.41 (d, 3H, J=6.4 Hz), 1.18 (s, 3H), 1.14 (s, 3H); ^{13}C NMR ($CDCl_3$, 50 MHz) δ 169.88, 166.65, 147.22, 137.84, 128.71, 125.98, 121.12, 120.07, 69.84, 67.75, 59.31, 51.88, 47.10, 39.84, 29.62, 28.69, 26.52, 21.06, 20.54, 19.71.

7b: ^{1}H NMR ($CDCl_3$, 200 MHz) δ 7.41-7.22 (m, 3H), 7.20-7.14 (m, 2H), 5.70 (d, 1H, J=1.2 Hz), 5.67 (s, 1H), 4.31-4.24 (m, 2H), 2.59-2.48 (m, 1H), 2.33-2.23 (m, 1H), 2.04-1.81 (m, 3H), 1.79-1.59 (m, 3H), 1.50-1.29 9 (m, 3H), 1.17 (s, 3H), 1.13 (s, 3H), 0.99 (t, 3H, J=7.4 Hz); ^{13}C NMR ($CDCl_3$, 50 MHz) δ 169.88, 167.62, 146.11, 138.05, 128.69, 125.89, 121.03, 120.68, 73.47, 69.37, 59.29, 52.18, 46.94, 40.03, 28.63, 28.19, 26.55, 20.47, 19.83, 10.06.

7c: ^{1}H NMR ($CDCl_3$, 200 MHz) δ 7.40-7.13 (m, 10H), 5.69 (d, 1H, J=1.0 Hz), 5.67 (s, 1H), 4.38 (dd, 1H, J=6.5, 6.5 Hz), 4.27 (dd, 1H, J=7.8, 4.8 Hz), 2.94-2.80 (m, 1H), 2.75-2.68 (m, 1H), 2.57-2.49 (m, 1H), 2.36-2.22 (m, 1H), 2.02-1.81 (m, 6H), 1.44-1.26 (m, 2H), 1.17 (s, 3H), 1.14 (s, 3H); ^{13}C NMR ($CDCl_3$, 50 MHz) δ 169.89, 167.26, 146.28, 141.57, 138.01, 128.68, 128.49, 128.45, 125.98, 125.90, 121.09, 120.61, 71.02, 69.48, 59.29, 52.07, 46.96, 39.89, 36.67, 31.80, 28.60, 26.51, 20.45, 19.79.

7d: ^{1}H NMR ($CDCl_3$, 200 MHz) δ 7.41-7.21 (m, 3H), 7.20-7.13 (m, 2H), 5.71 (d, 1H, J=1.2 Hz), 5.65 (s, 1H), 4.44 (dd, 1H, J=10.2, 3.6 Hz), 4.29 (dd, 1H, J=7.8, 5.2 Hz), 2.62-2.53 (m, 1H), 2.36-2.21 (m, 1H), 2.00-1.85 (m, 3H), 1.67-1.56 (m, 1H), 1.44-1.29 (m, 5H), 1.18 (s, 3H), 1.14 (s, 3H), 0.93 (d, 3H, J=6.6 Hz), 0.89 (d, 3H, J=6.6 Hz); ^{13}C NMR ($CDCl_3$, 50 MHz) δ 169.89, 167.46, 146.78, 138.02, 128.66, 125.87, 121.05, 120.36, 70.04, 69.46, 59.28, 52.09, 46.96, 44.23, 39.97, 28.63, 26.52, 24.26, 23.52, 21.27, 20.47, 19.80.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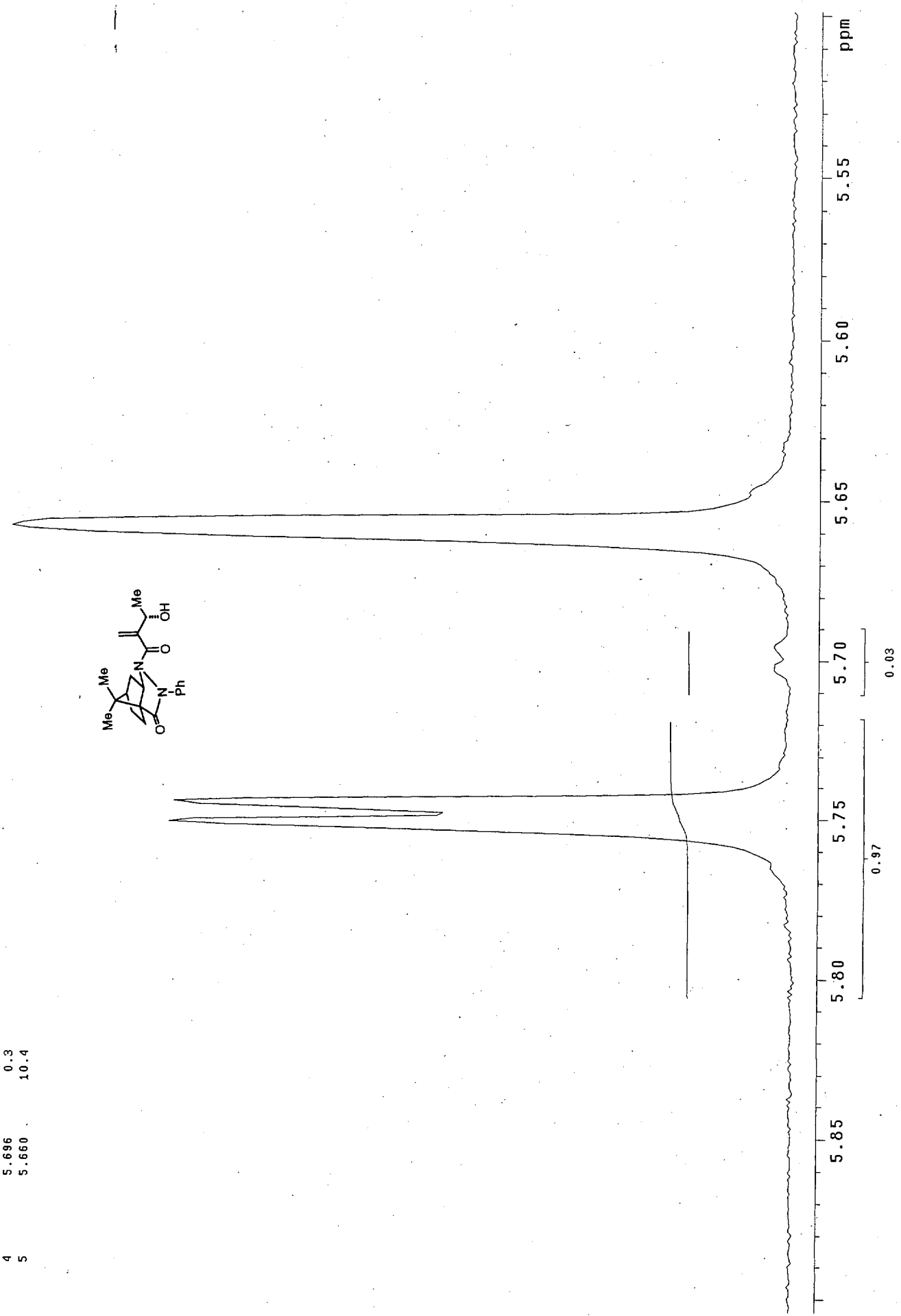
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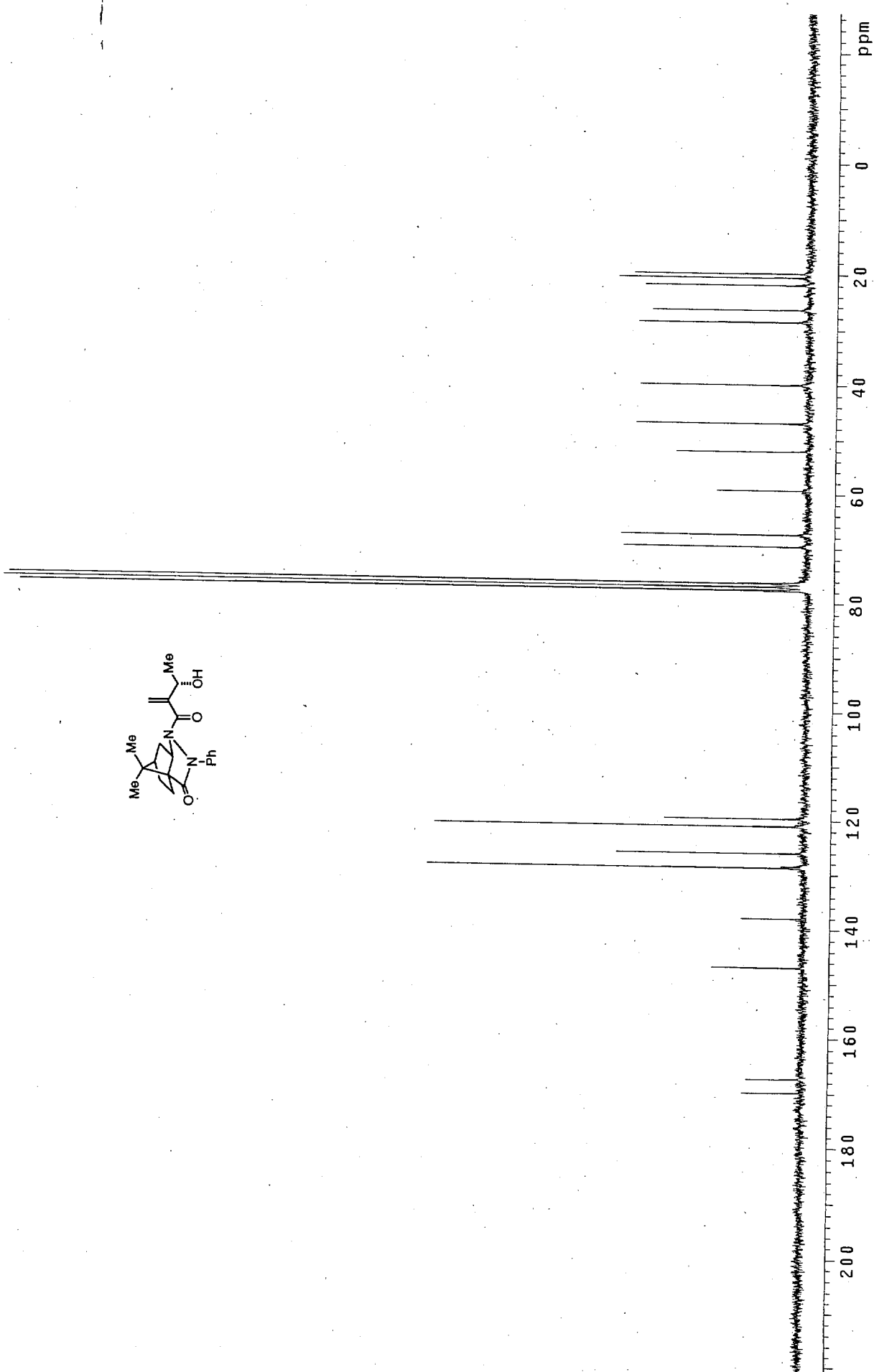

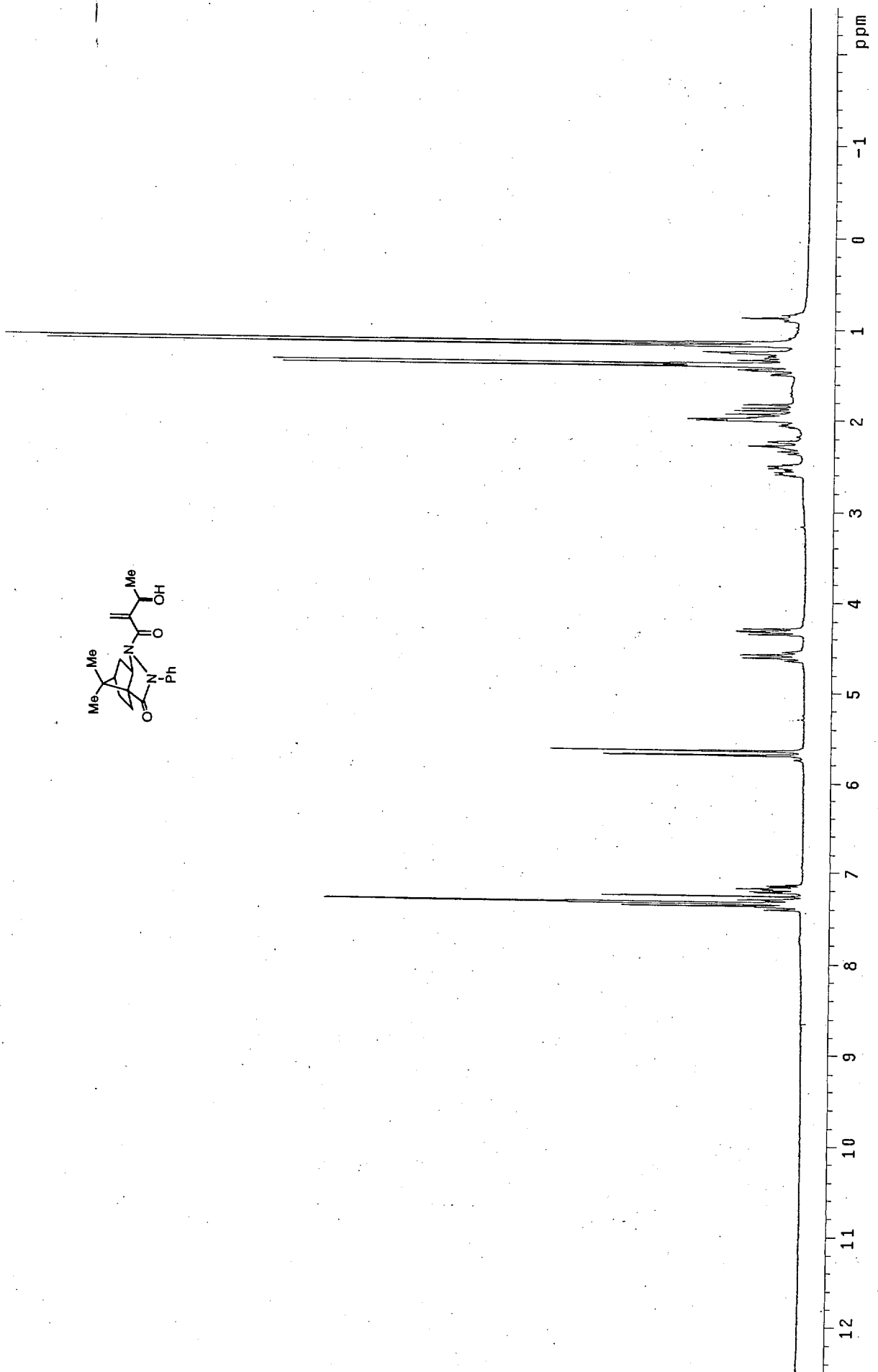

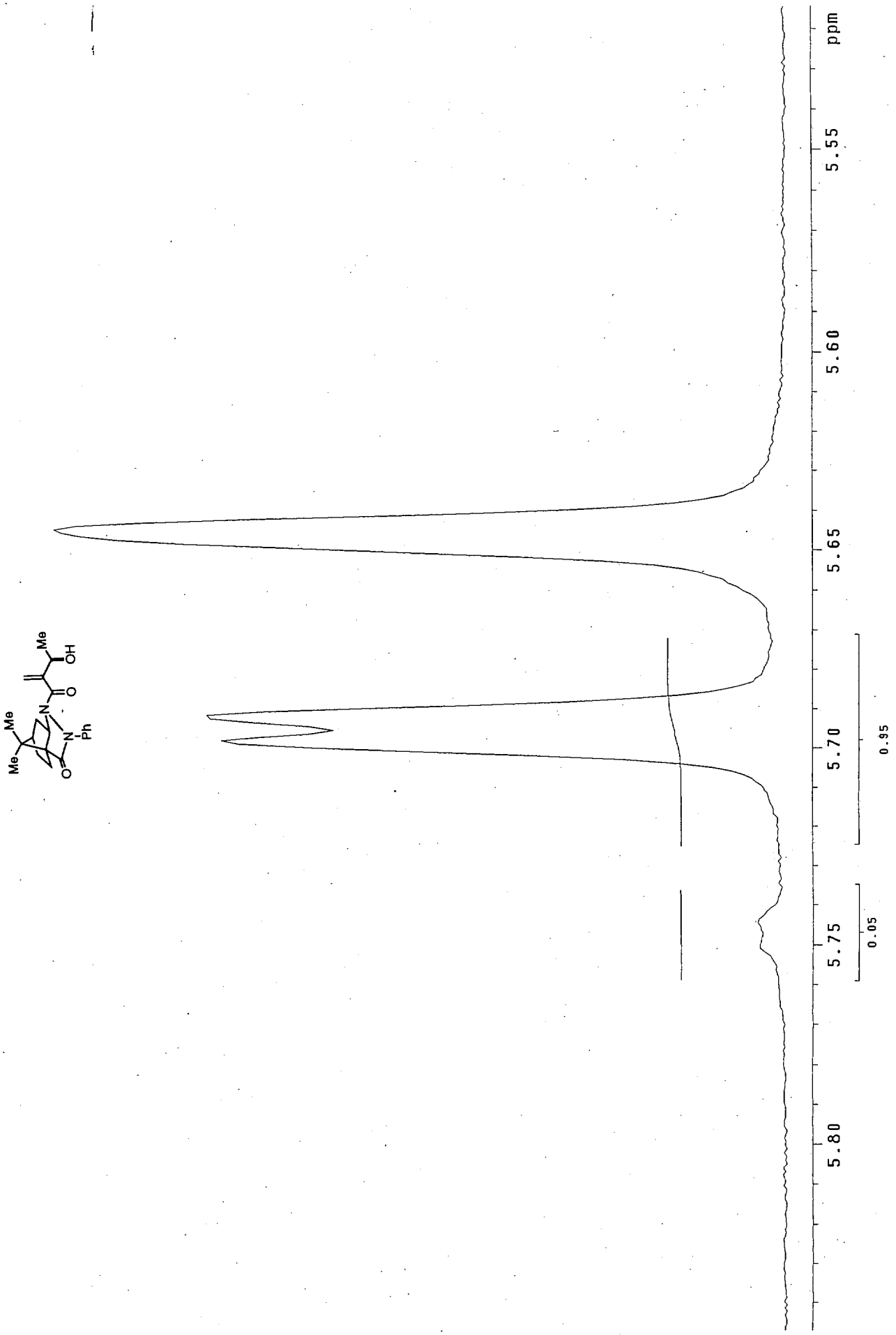
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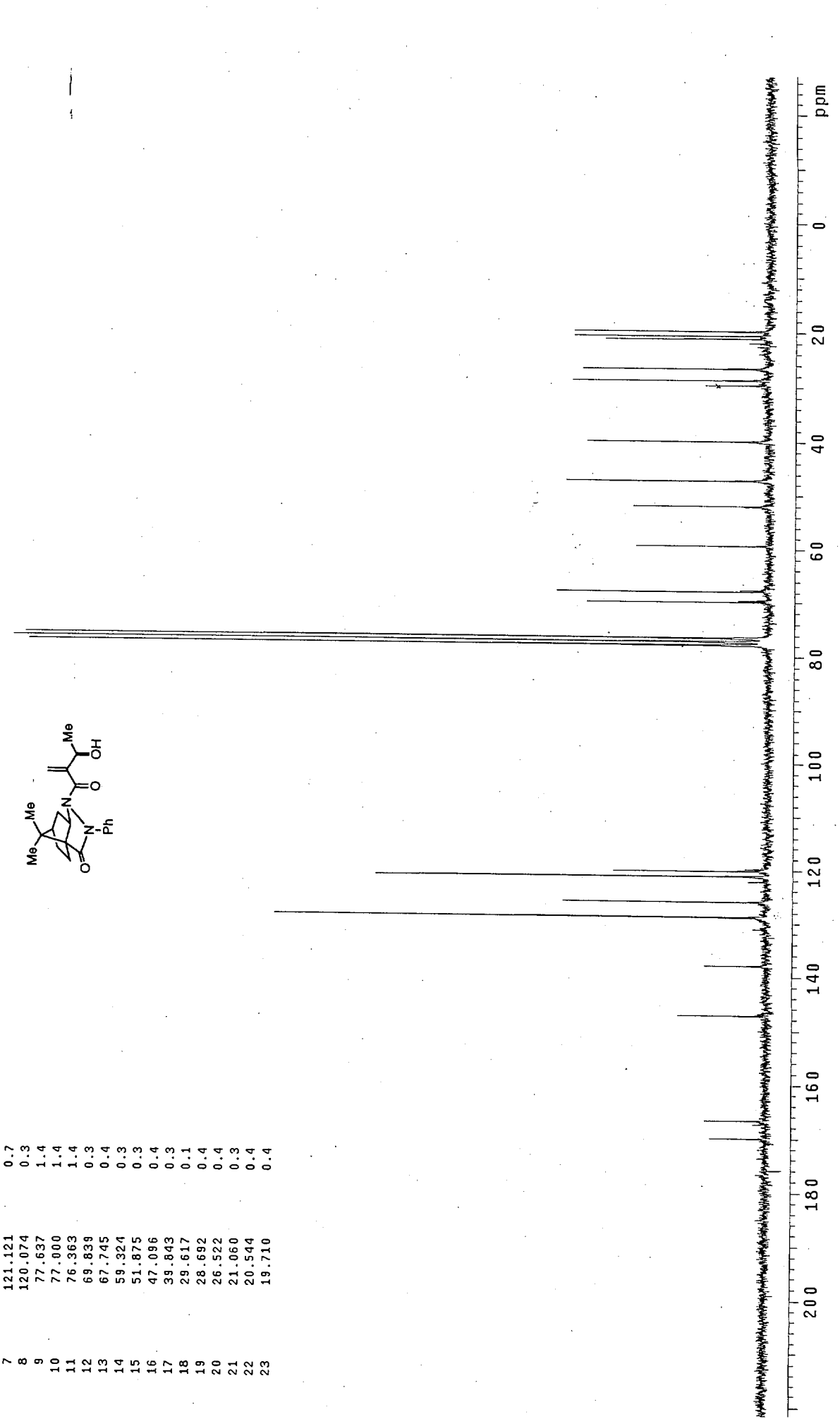

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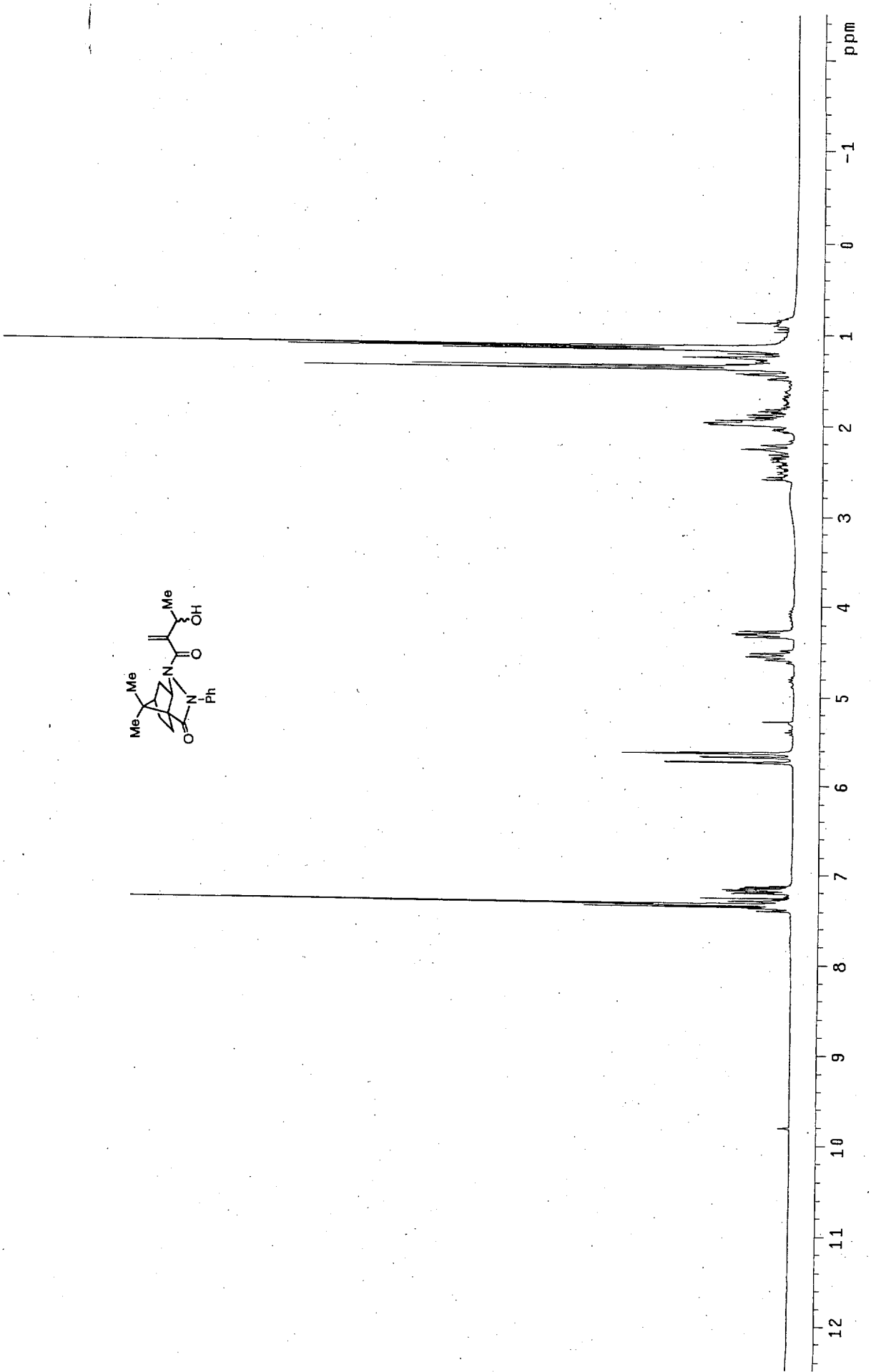

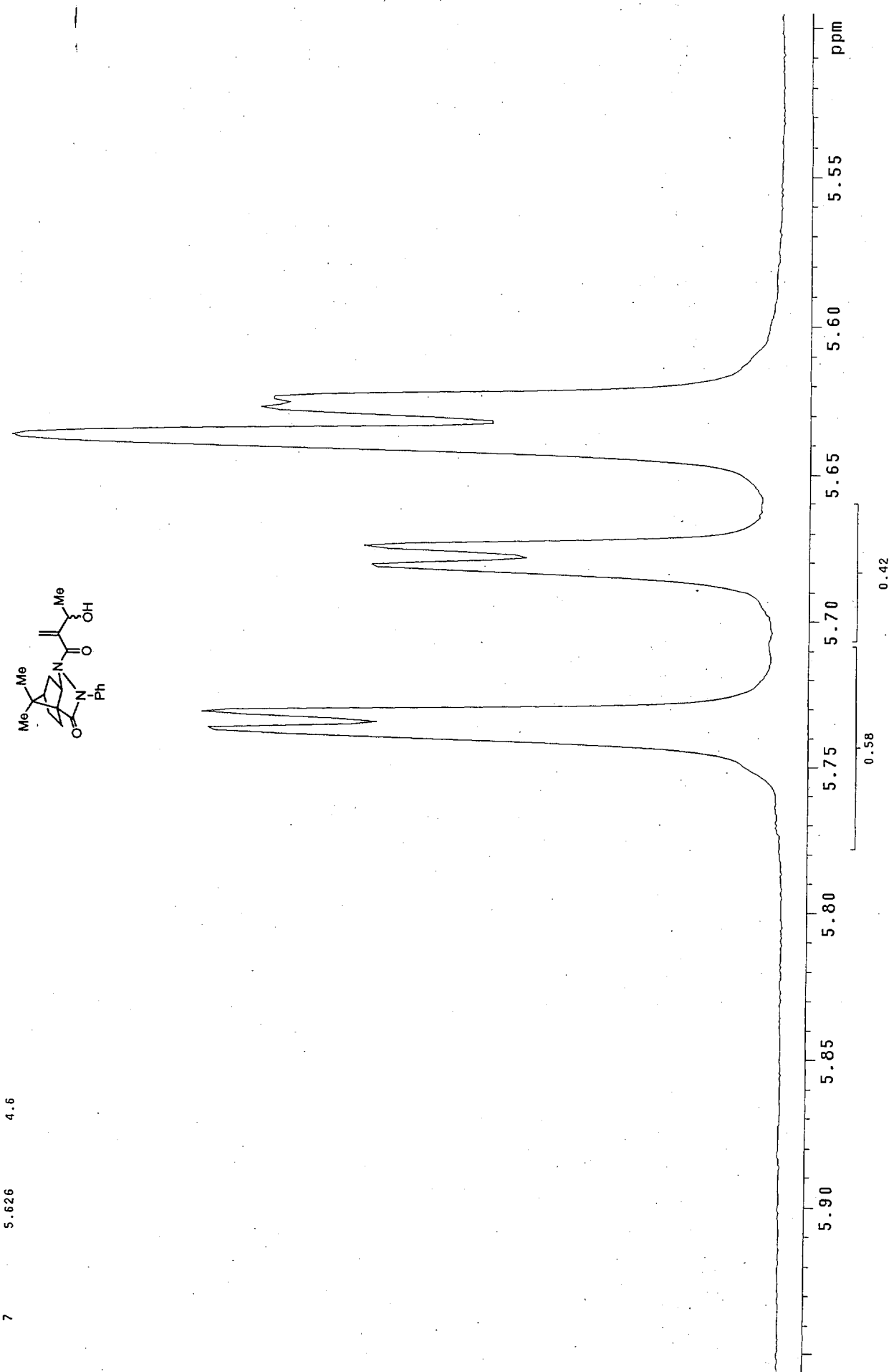

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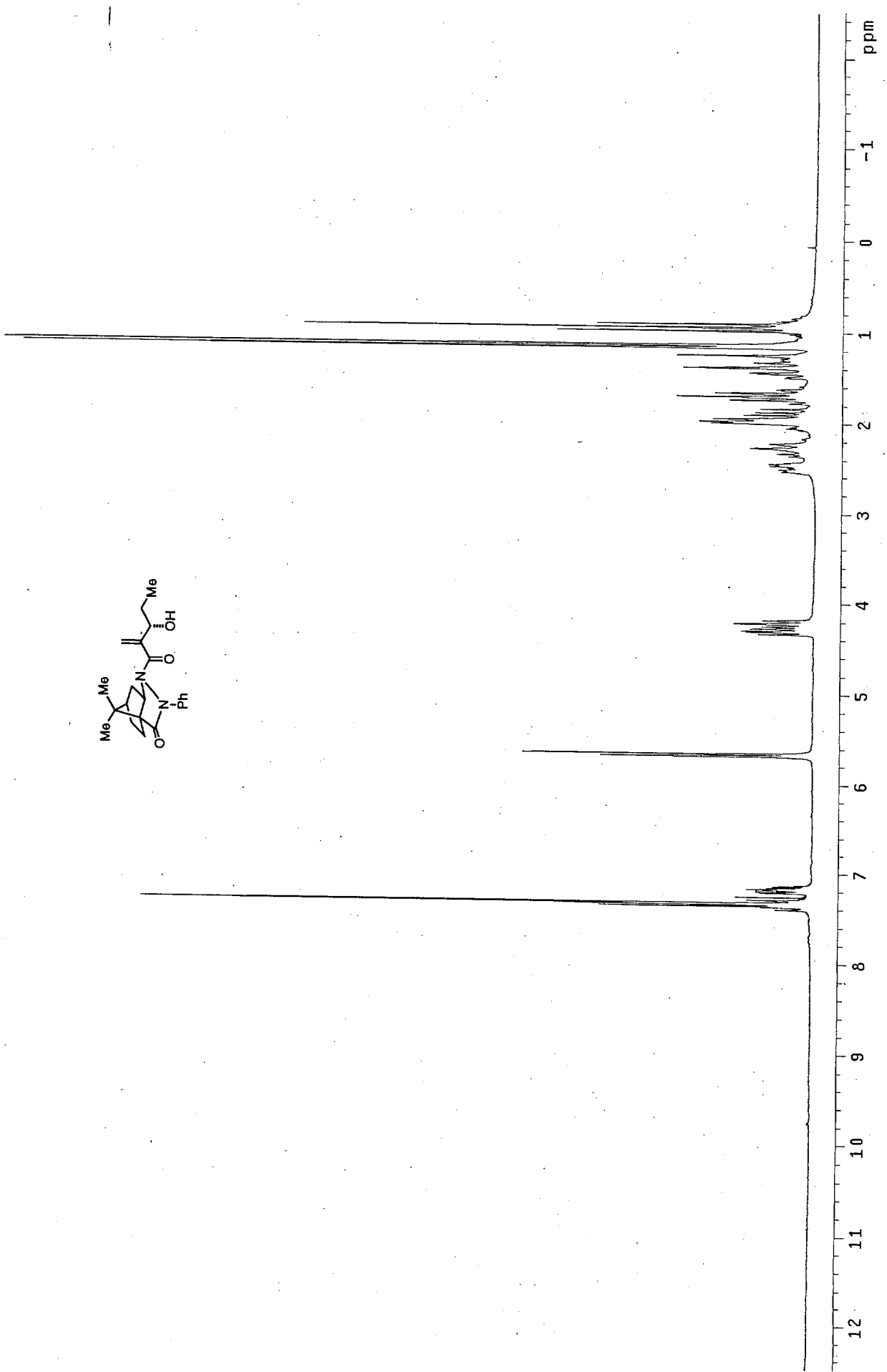

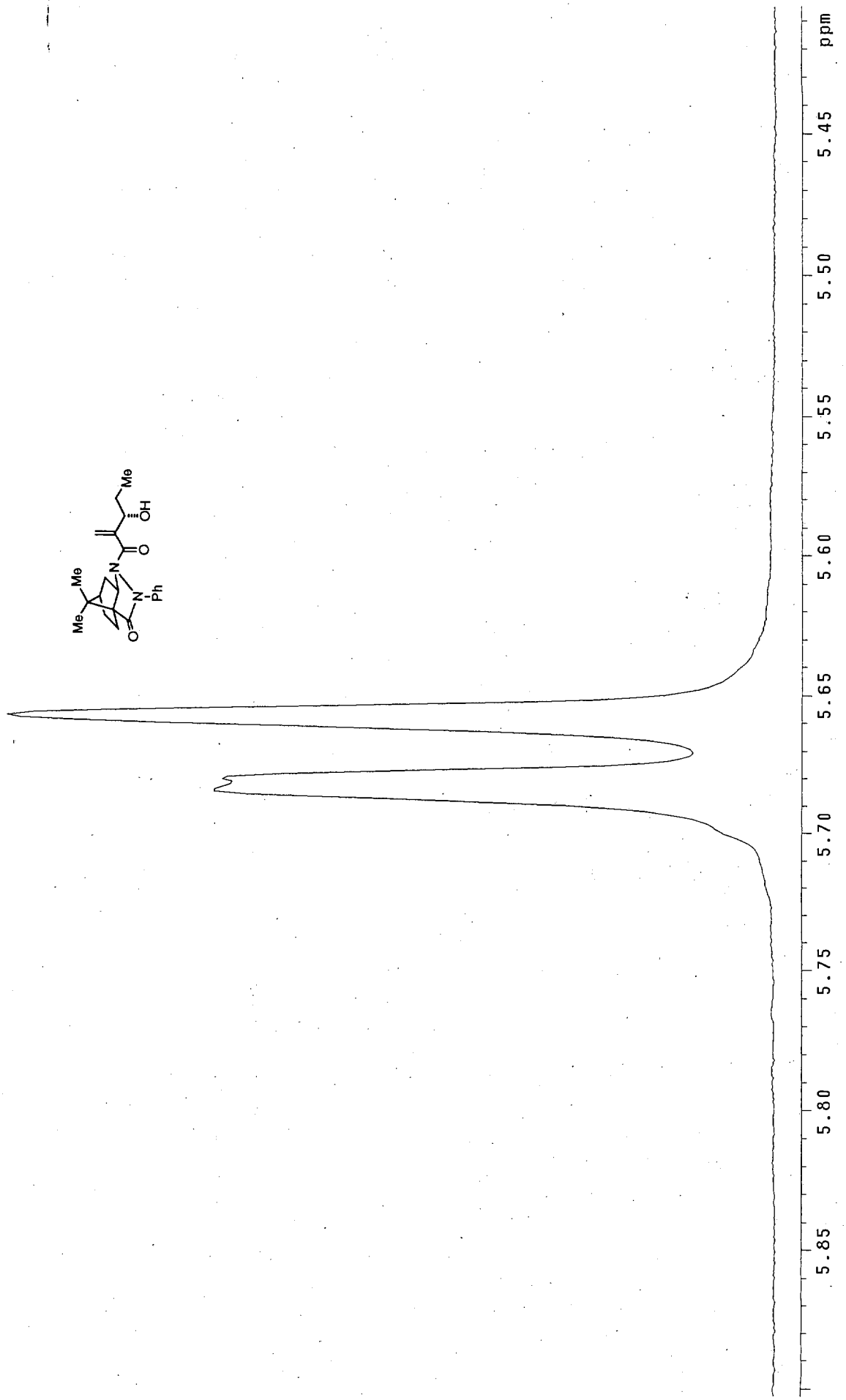

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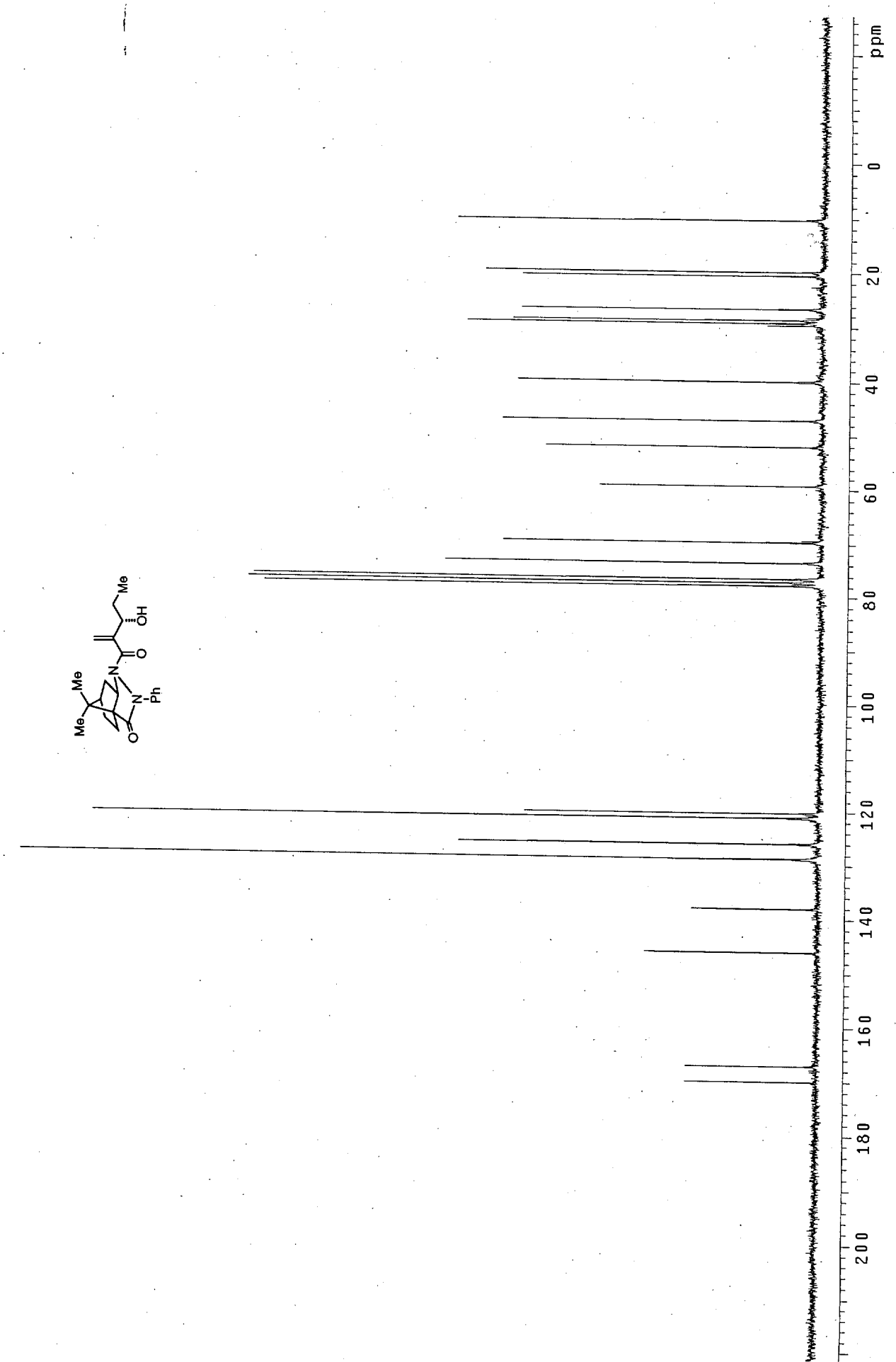
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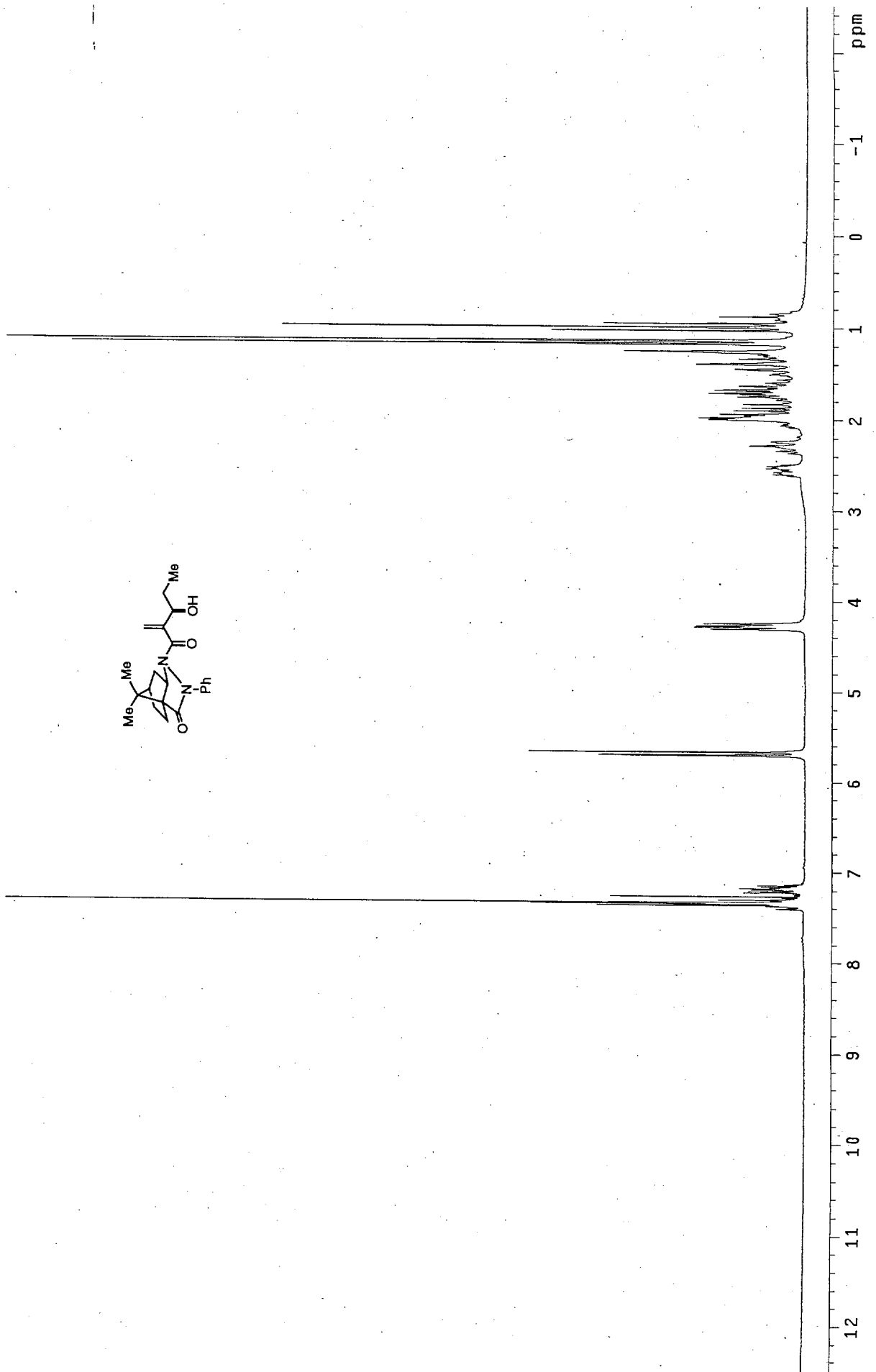
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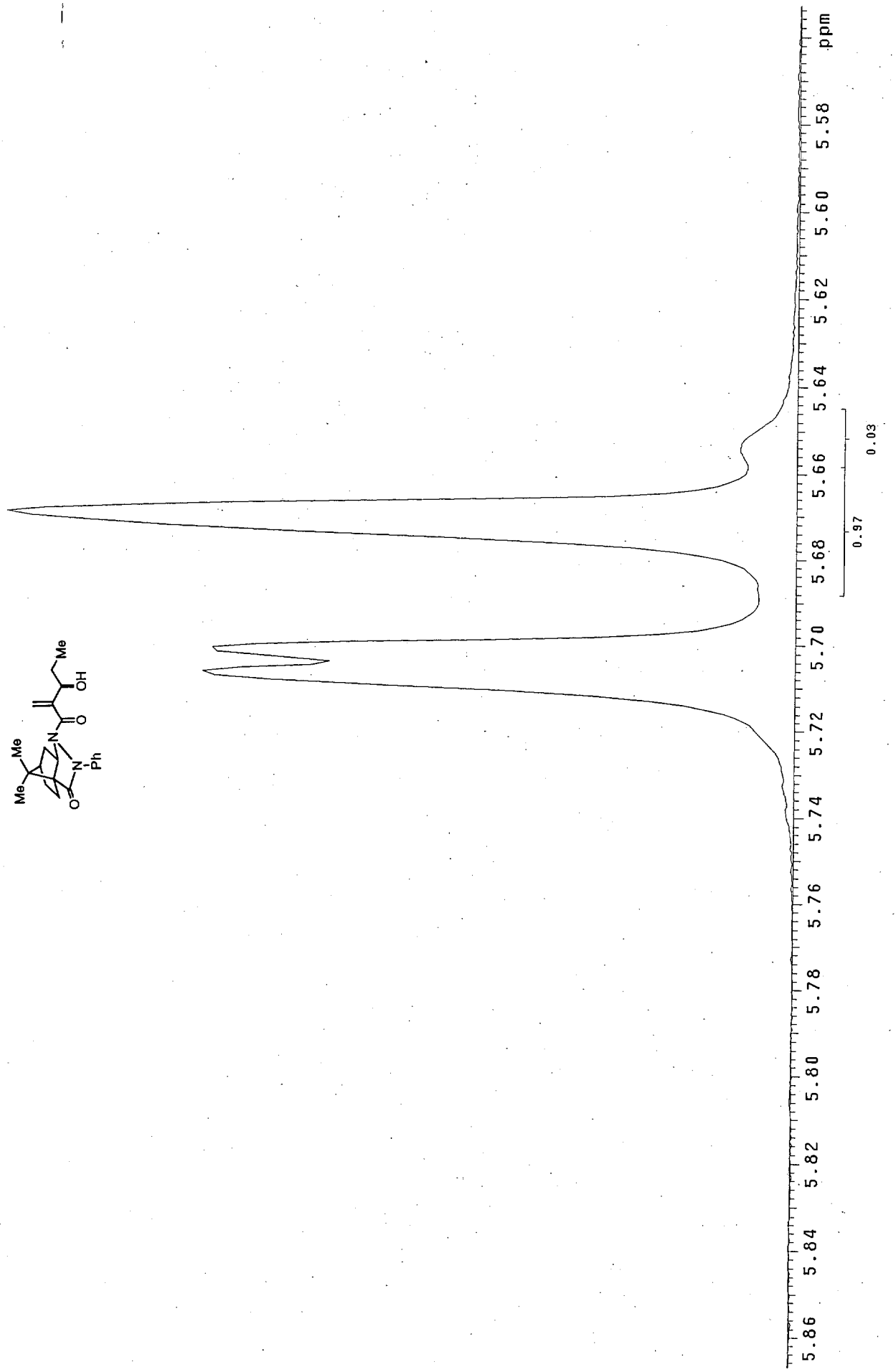

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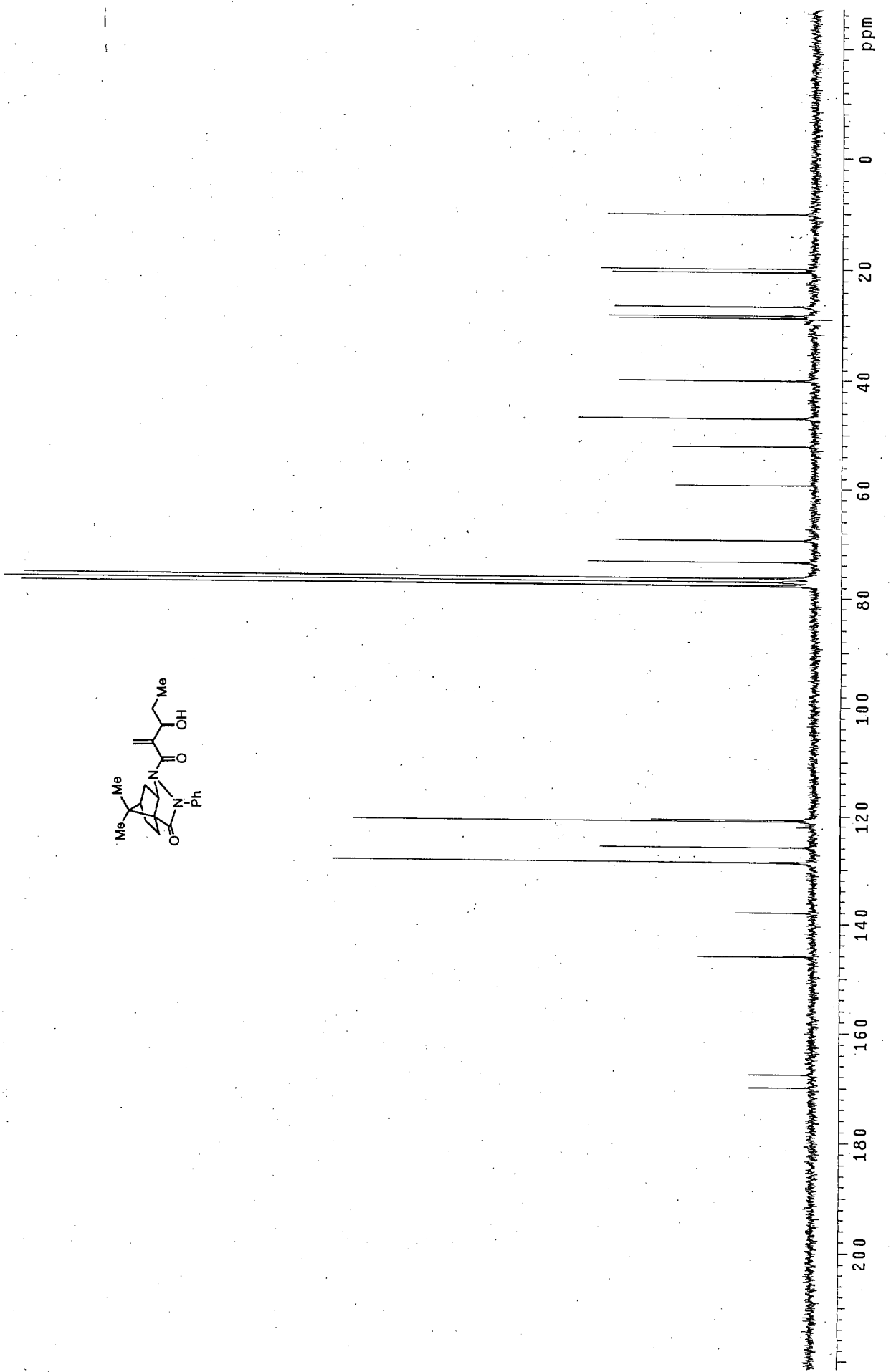

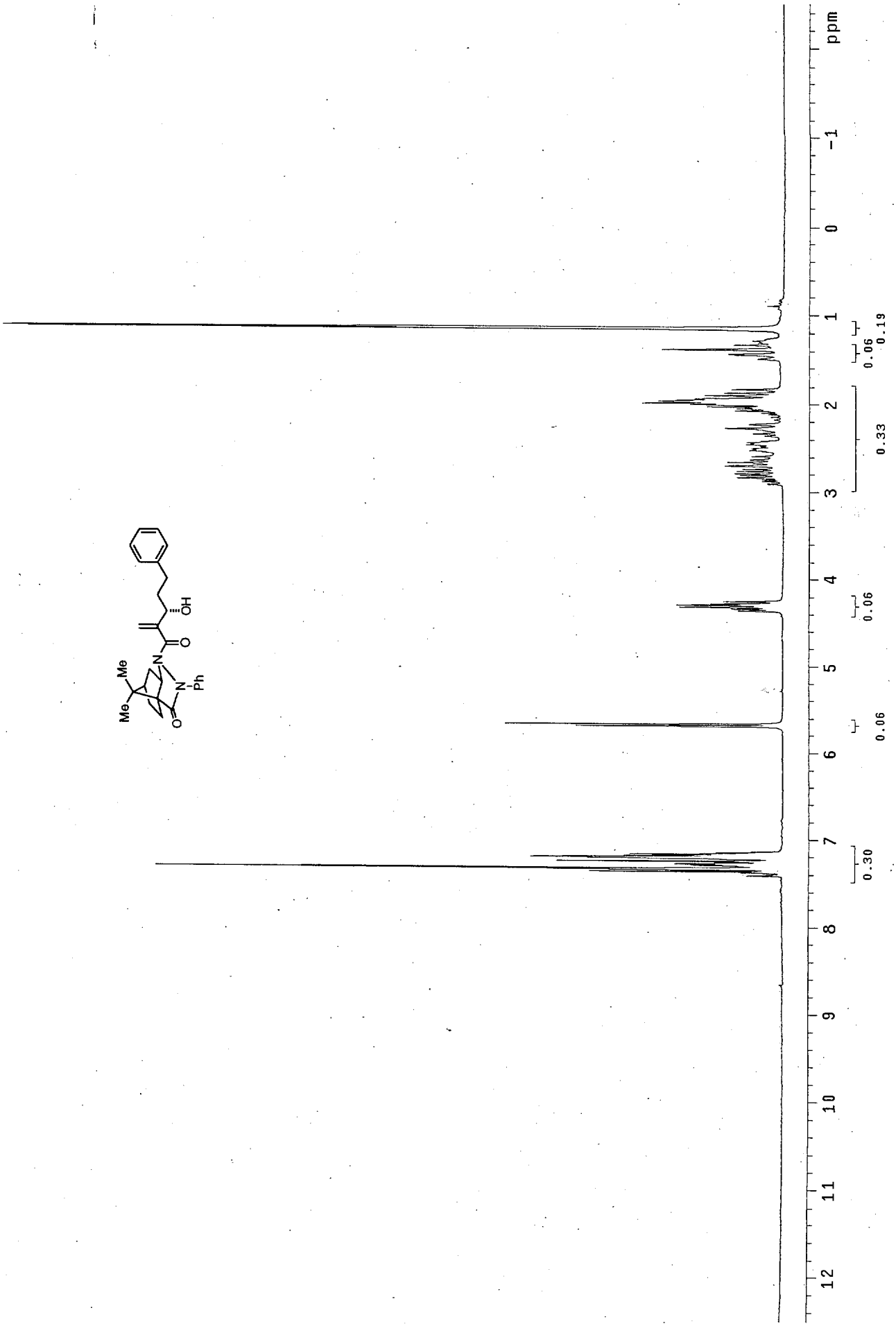
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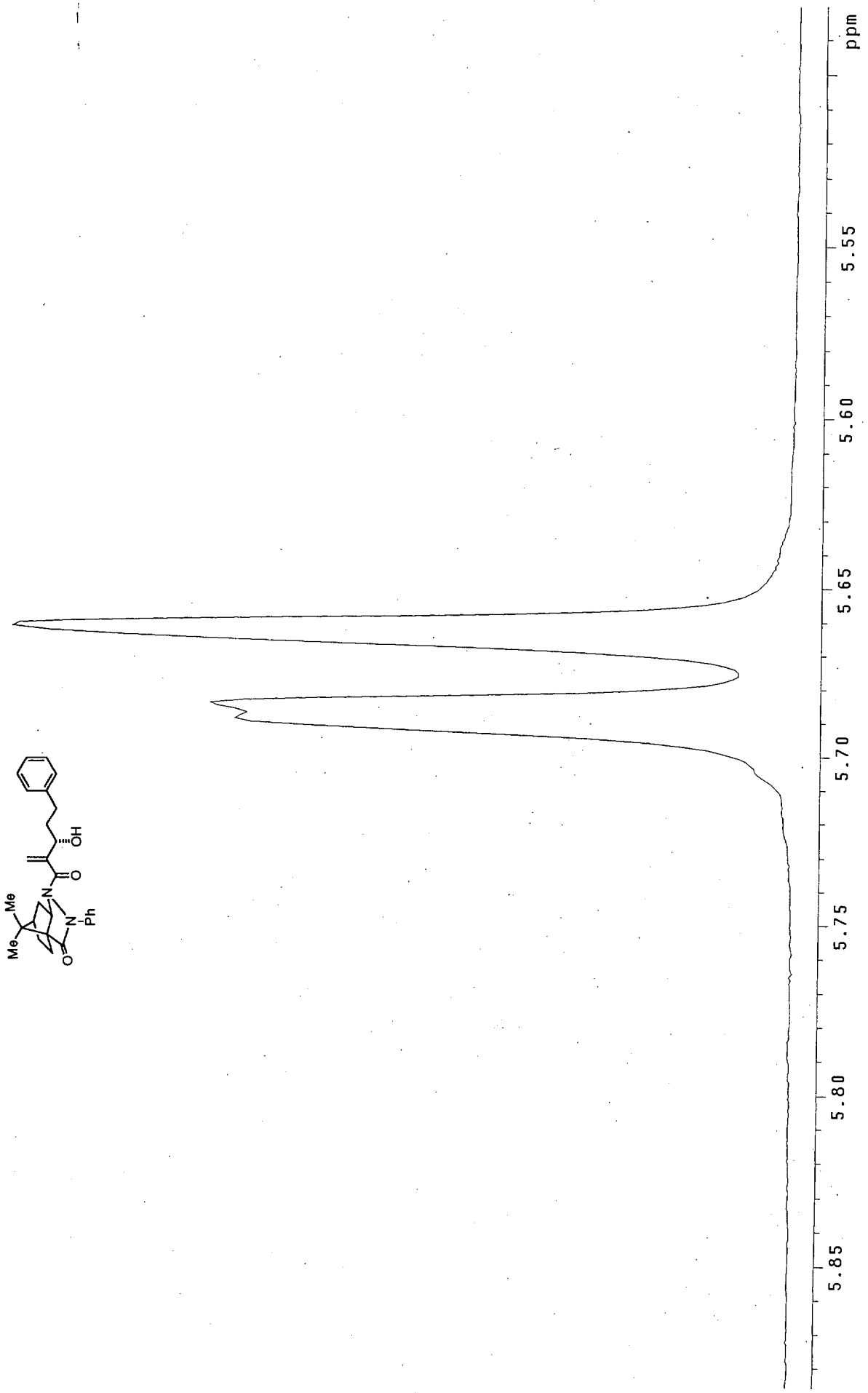
Ph
Me
Me
O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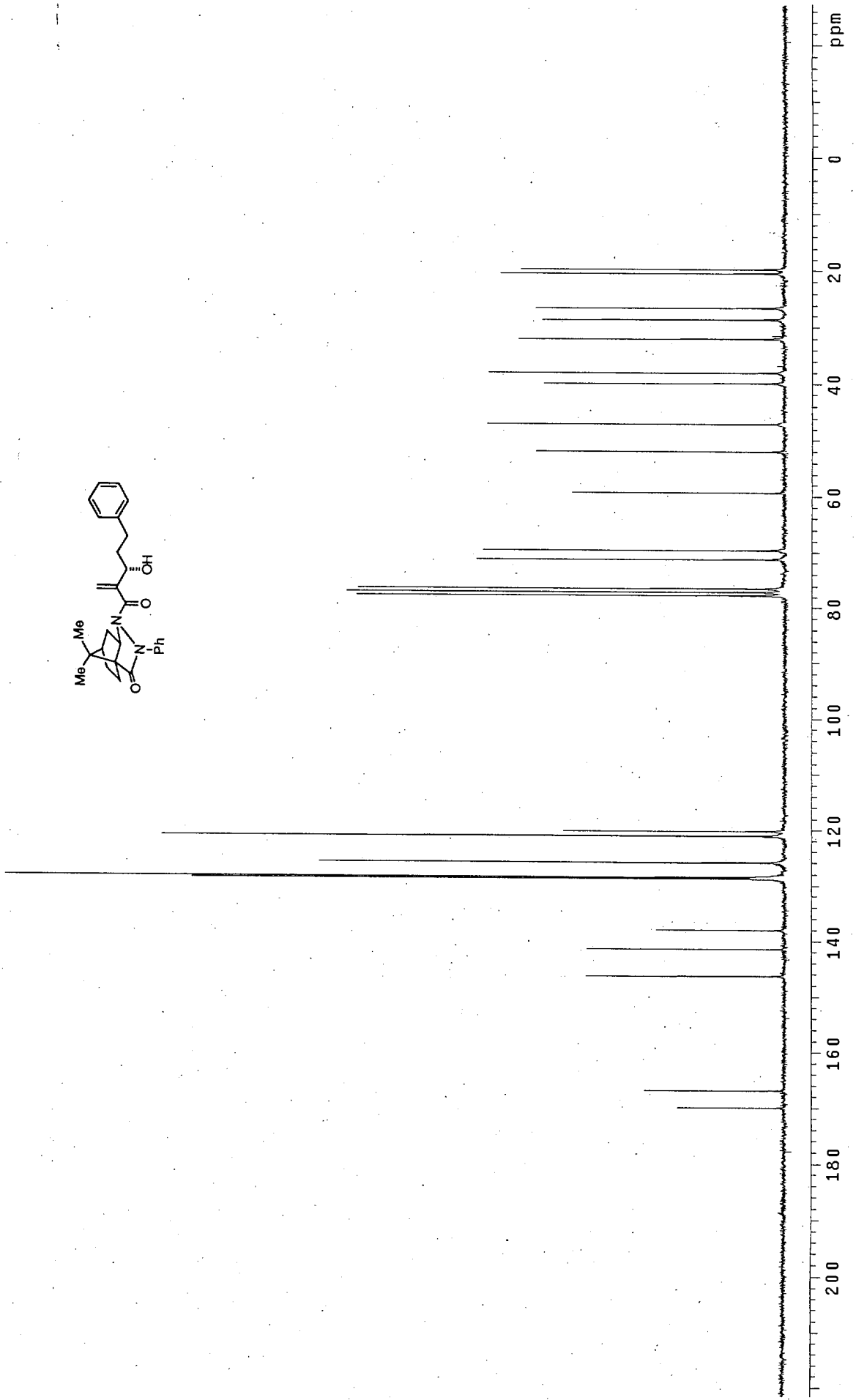
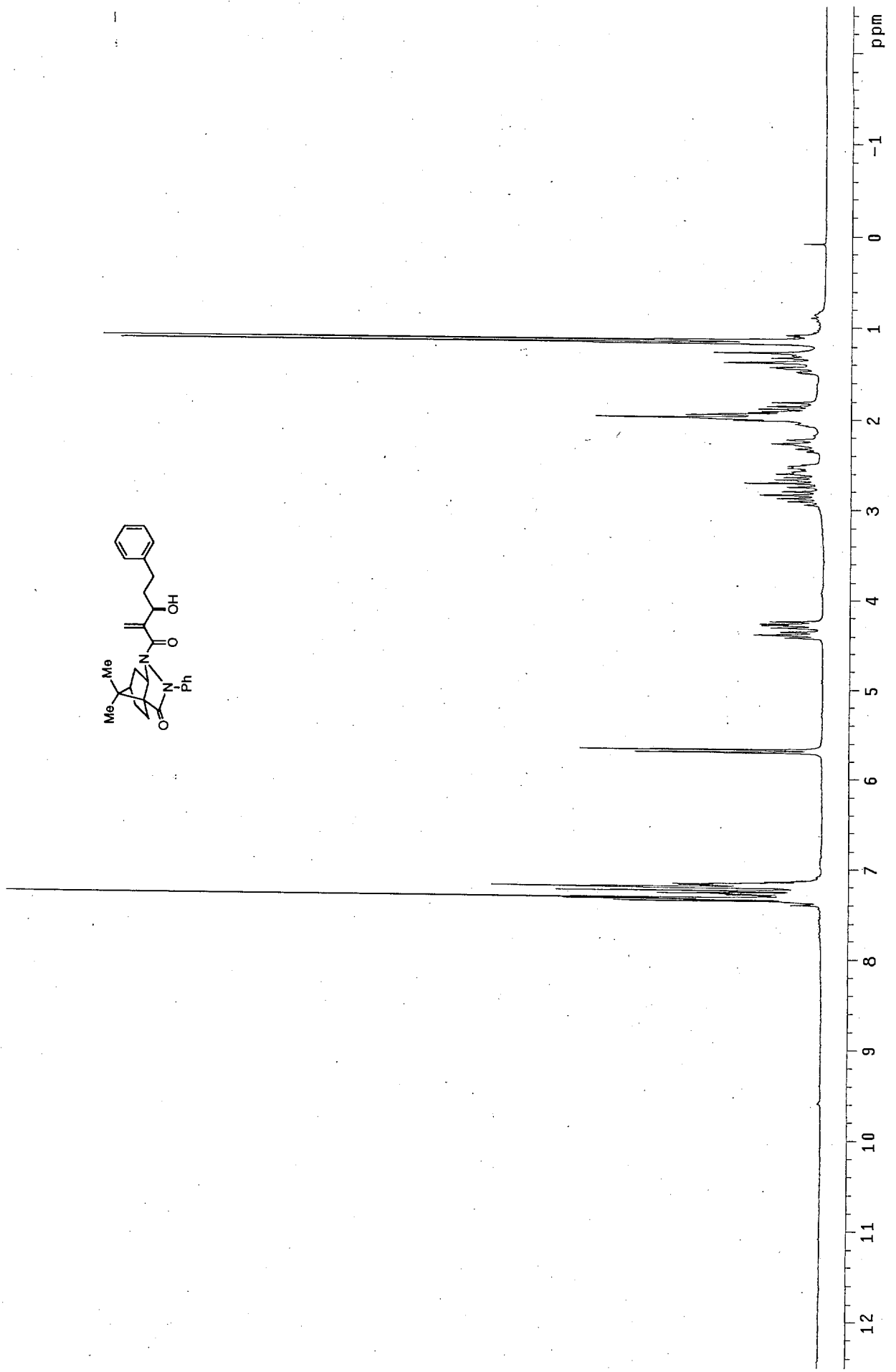
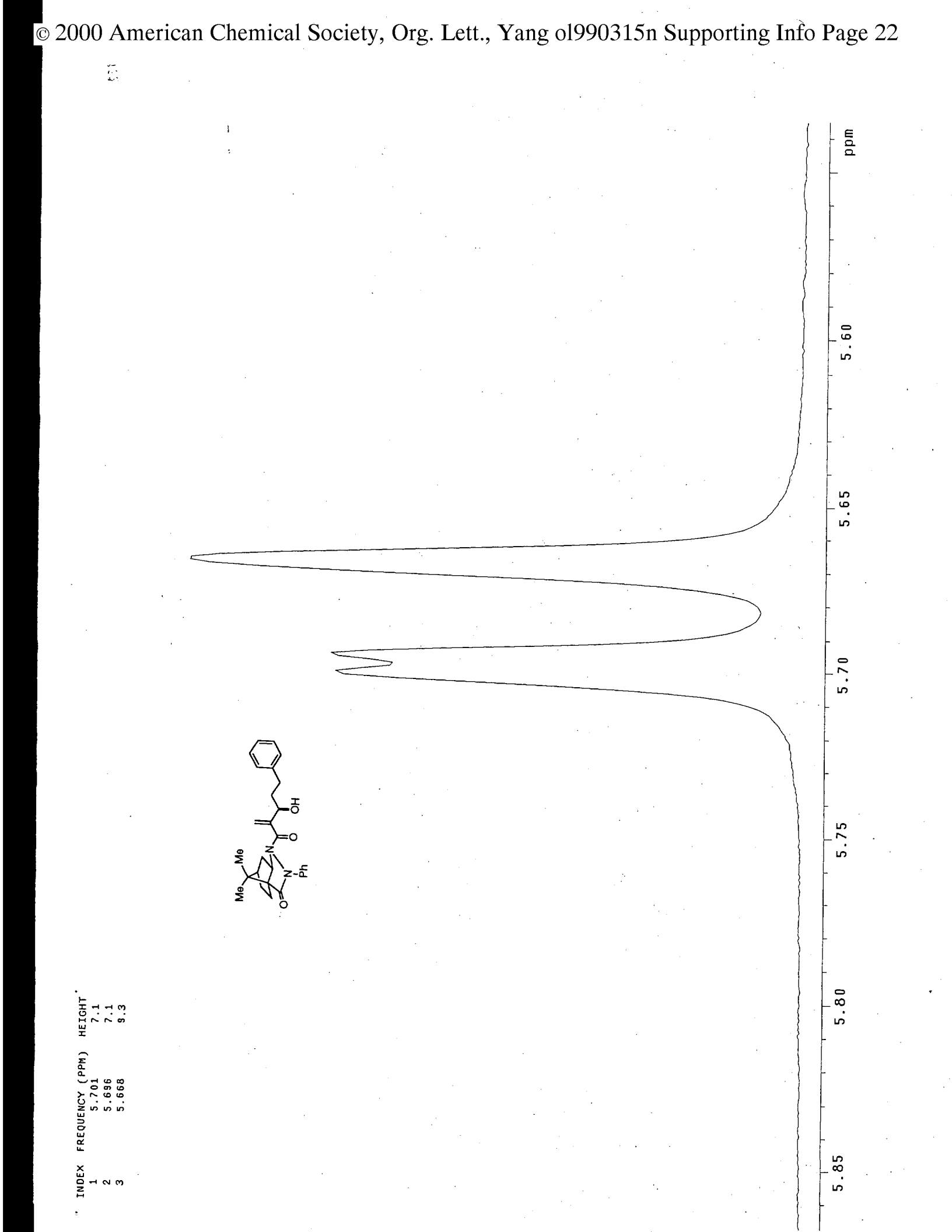
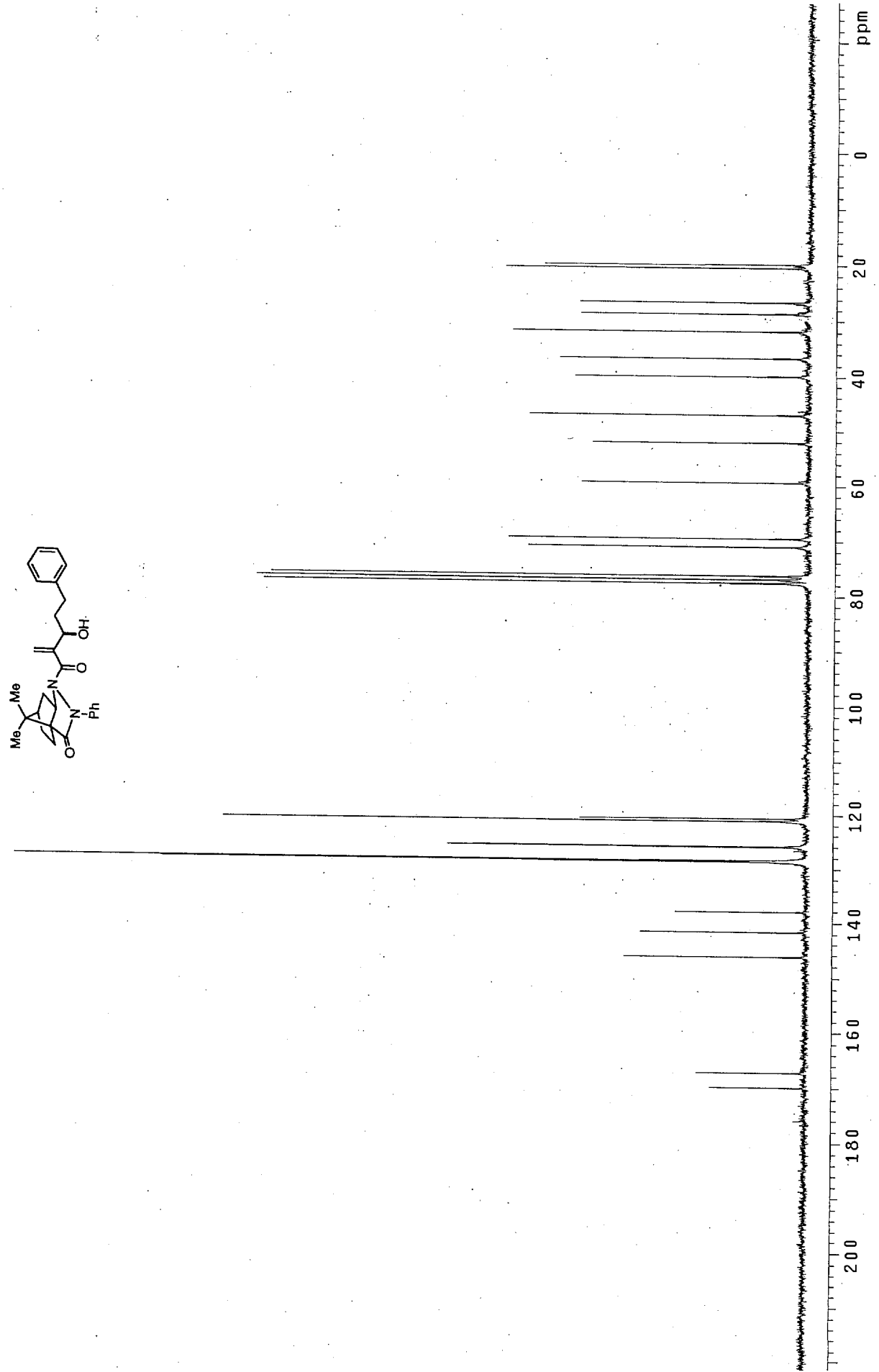
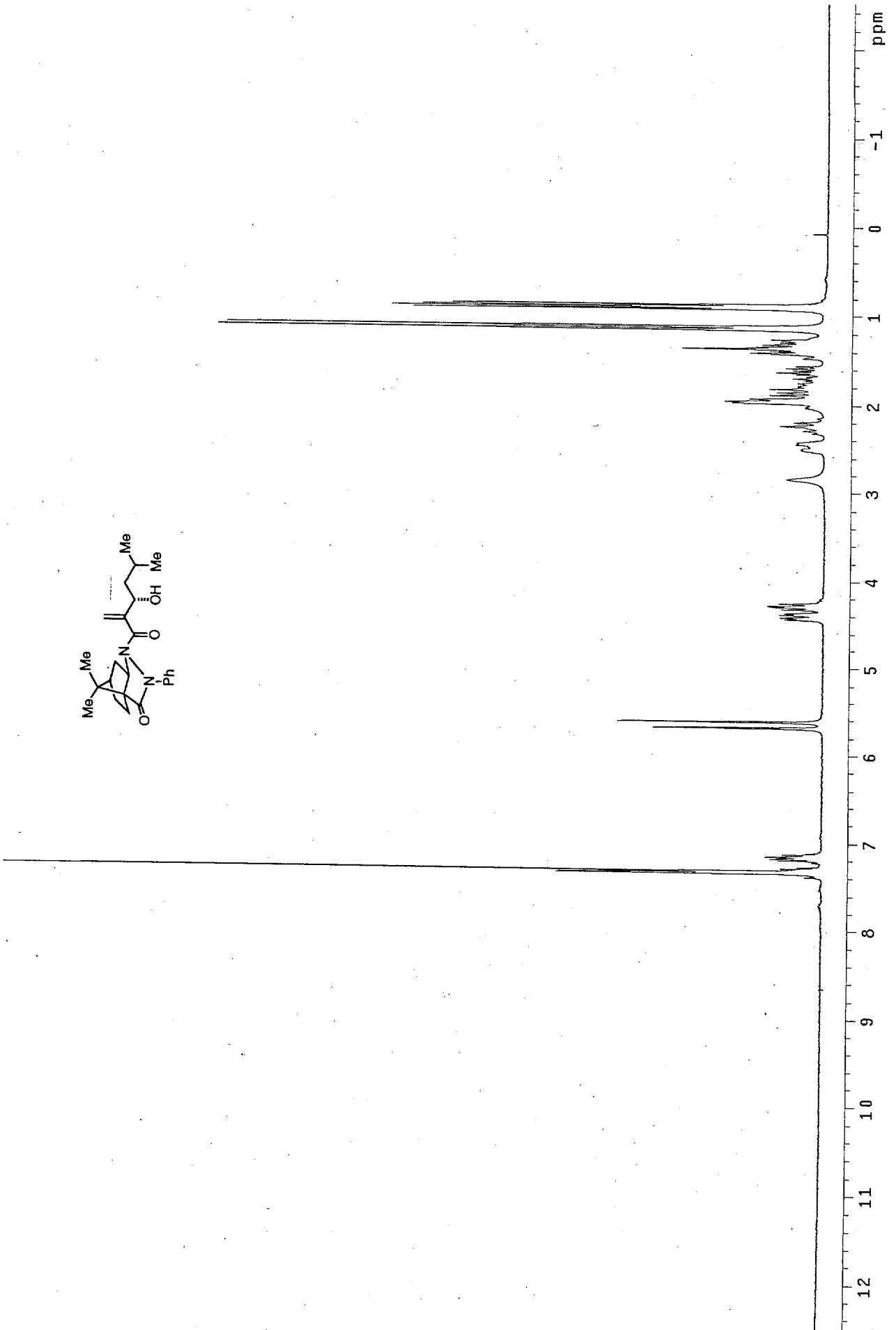
5.60
5.65
5.70
5.75
5.80
5.85
OH
O
N
Me
Me
N-Ph
O

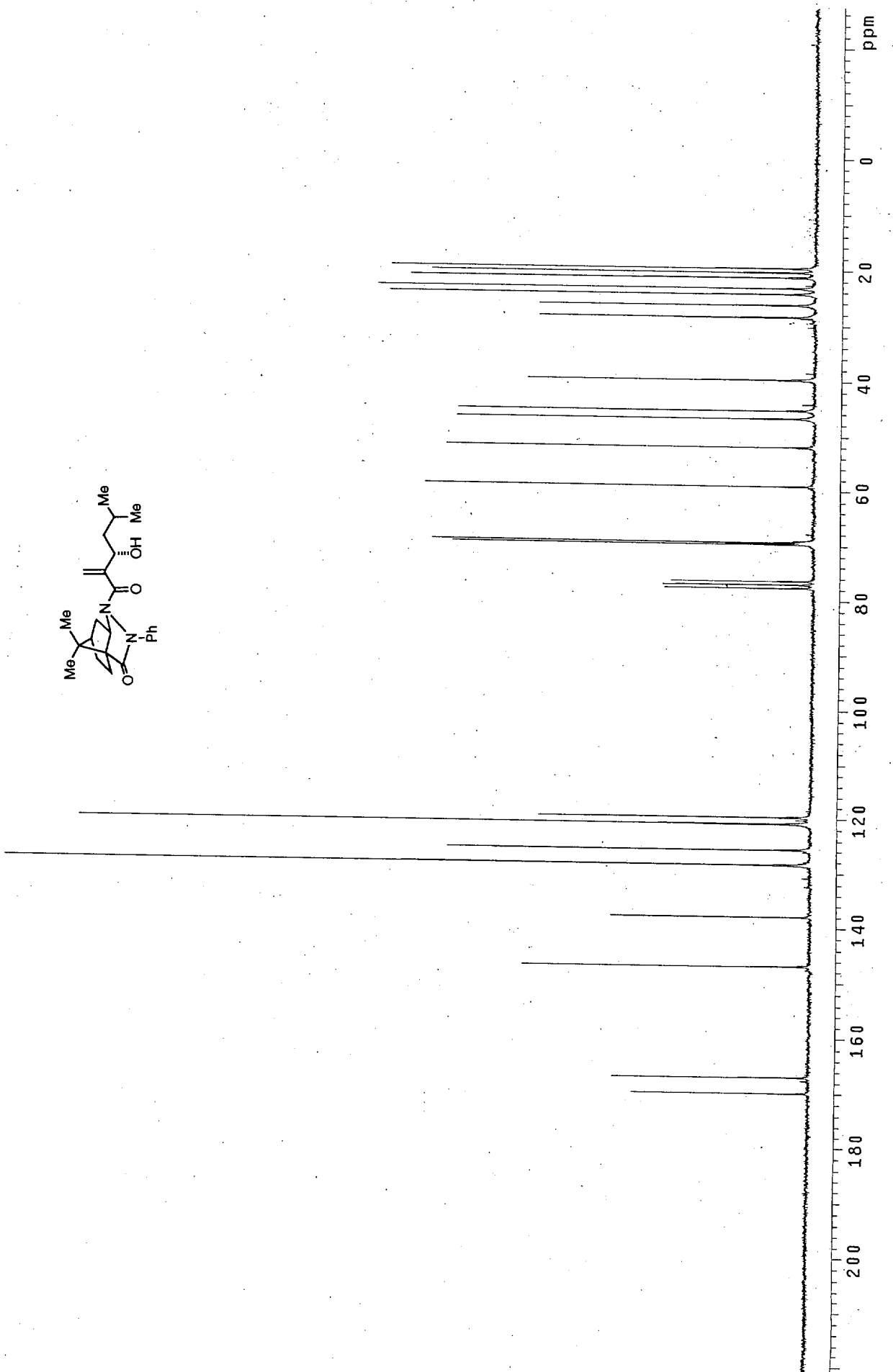


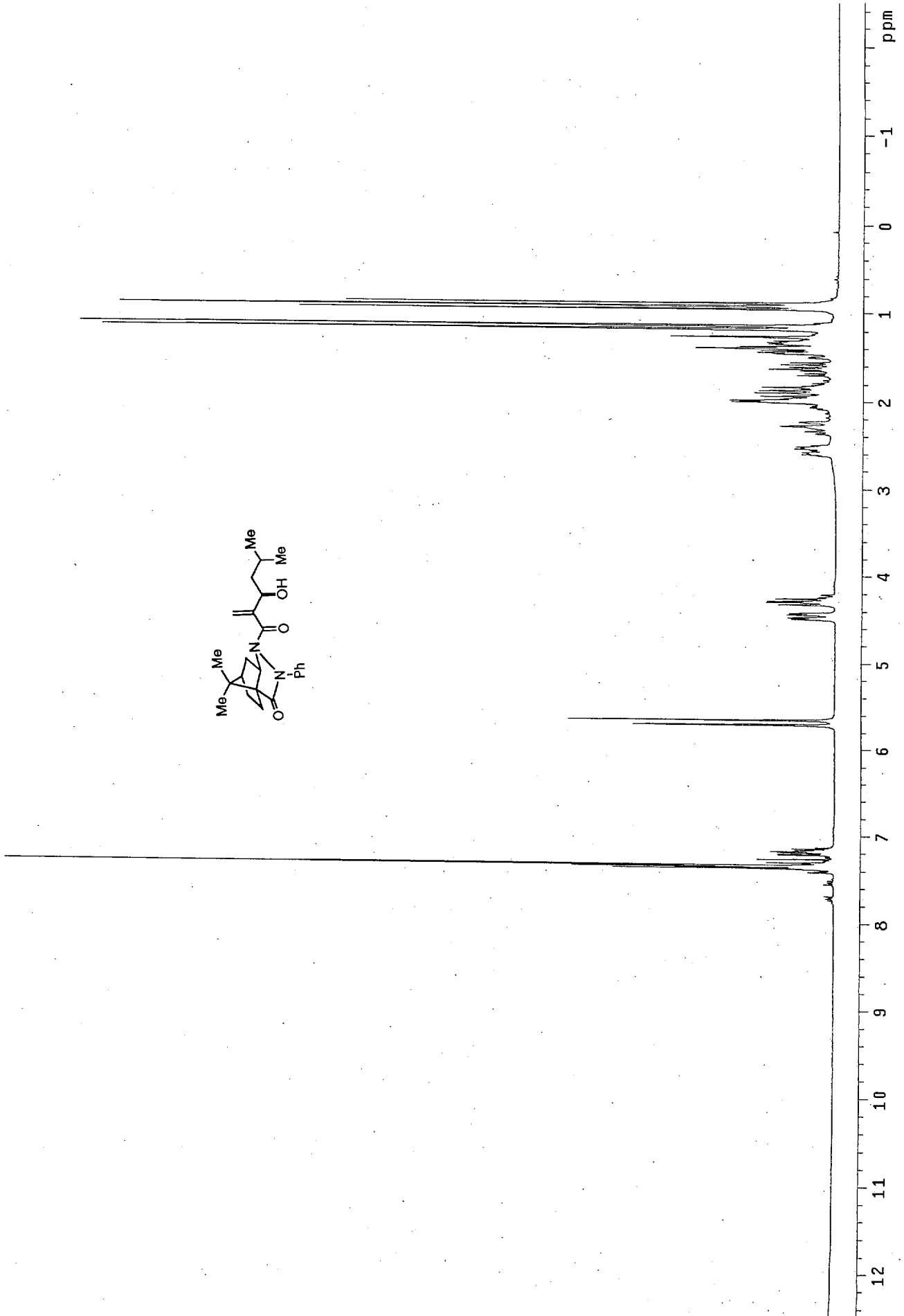


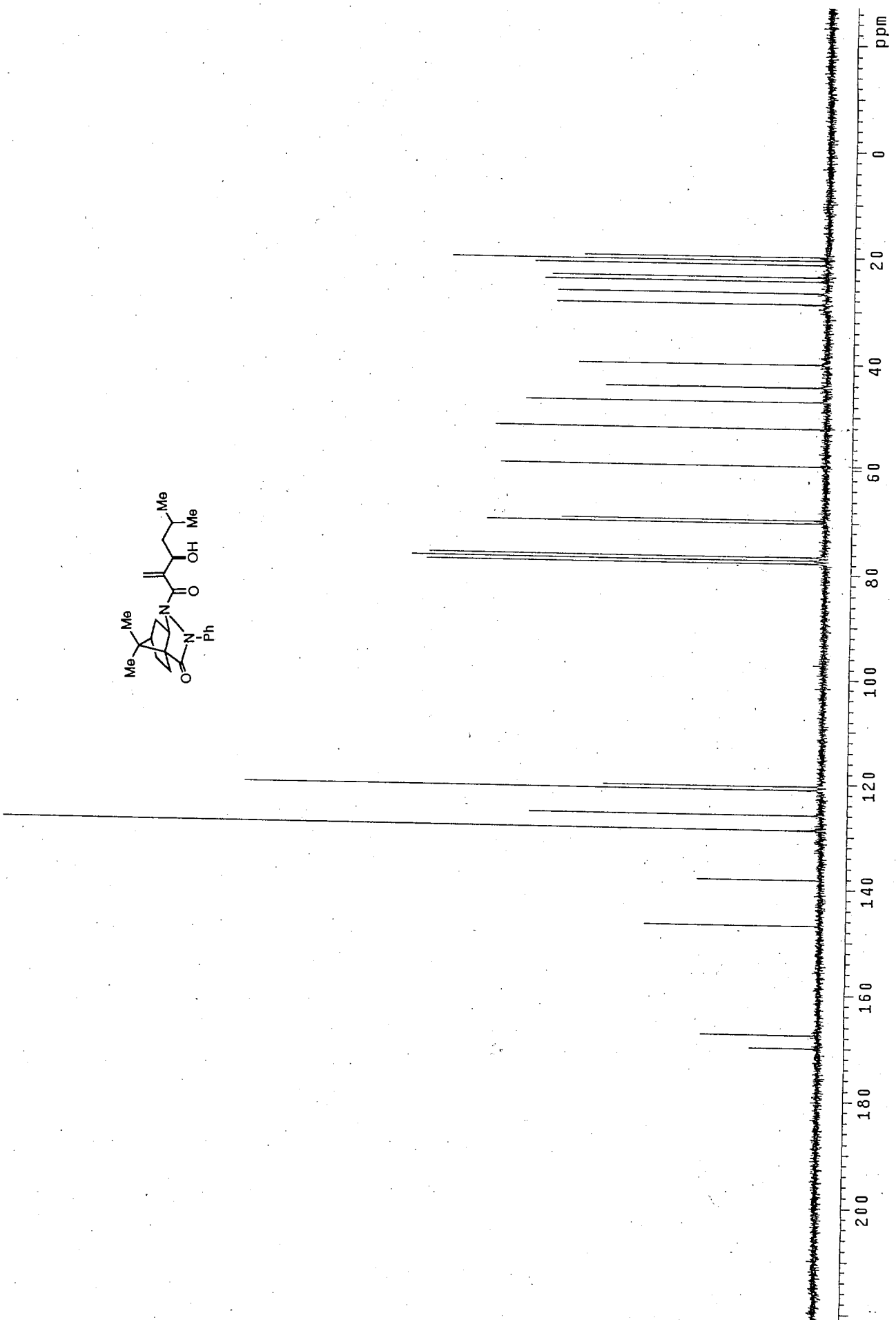


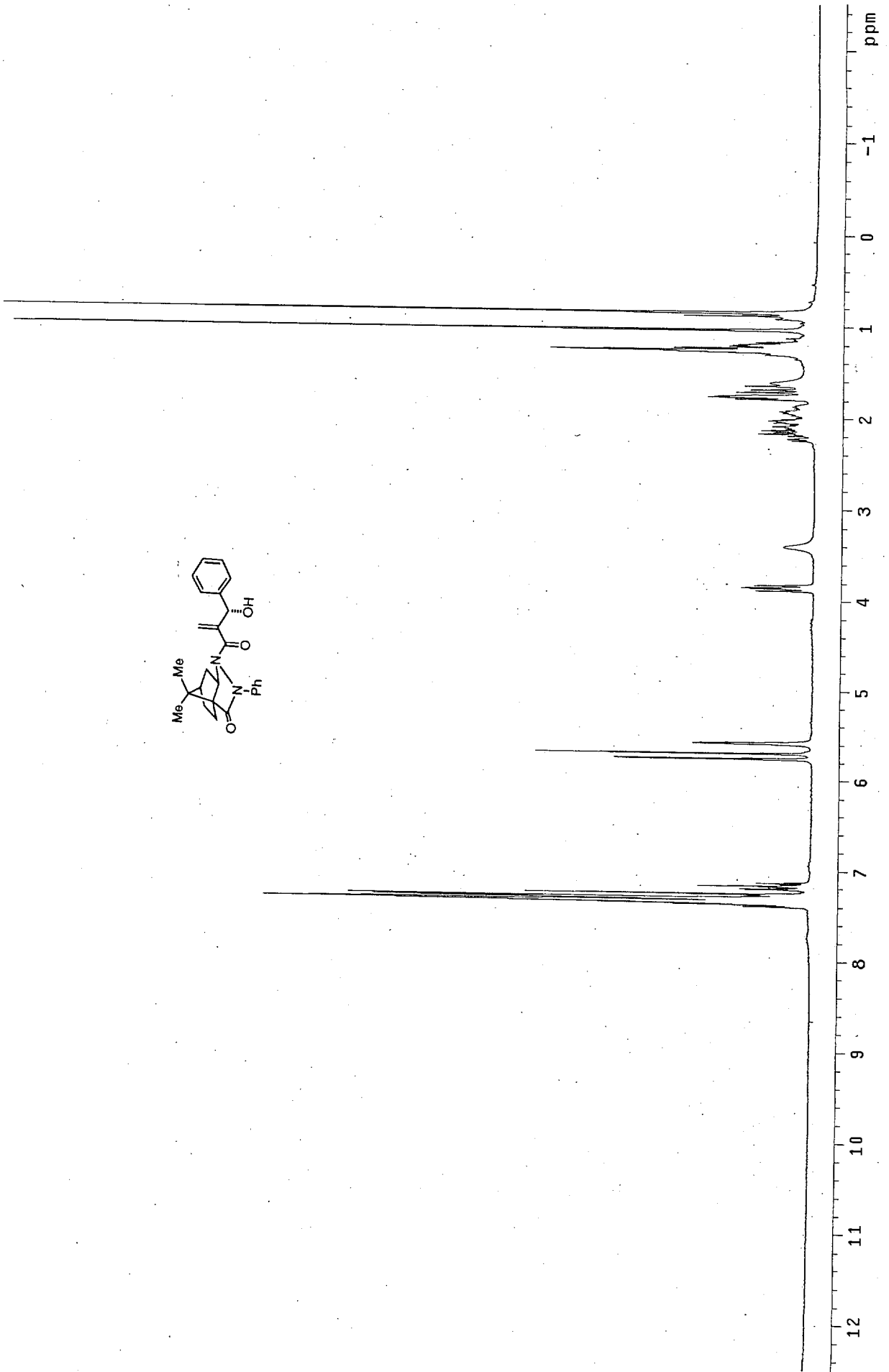












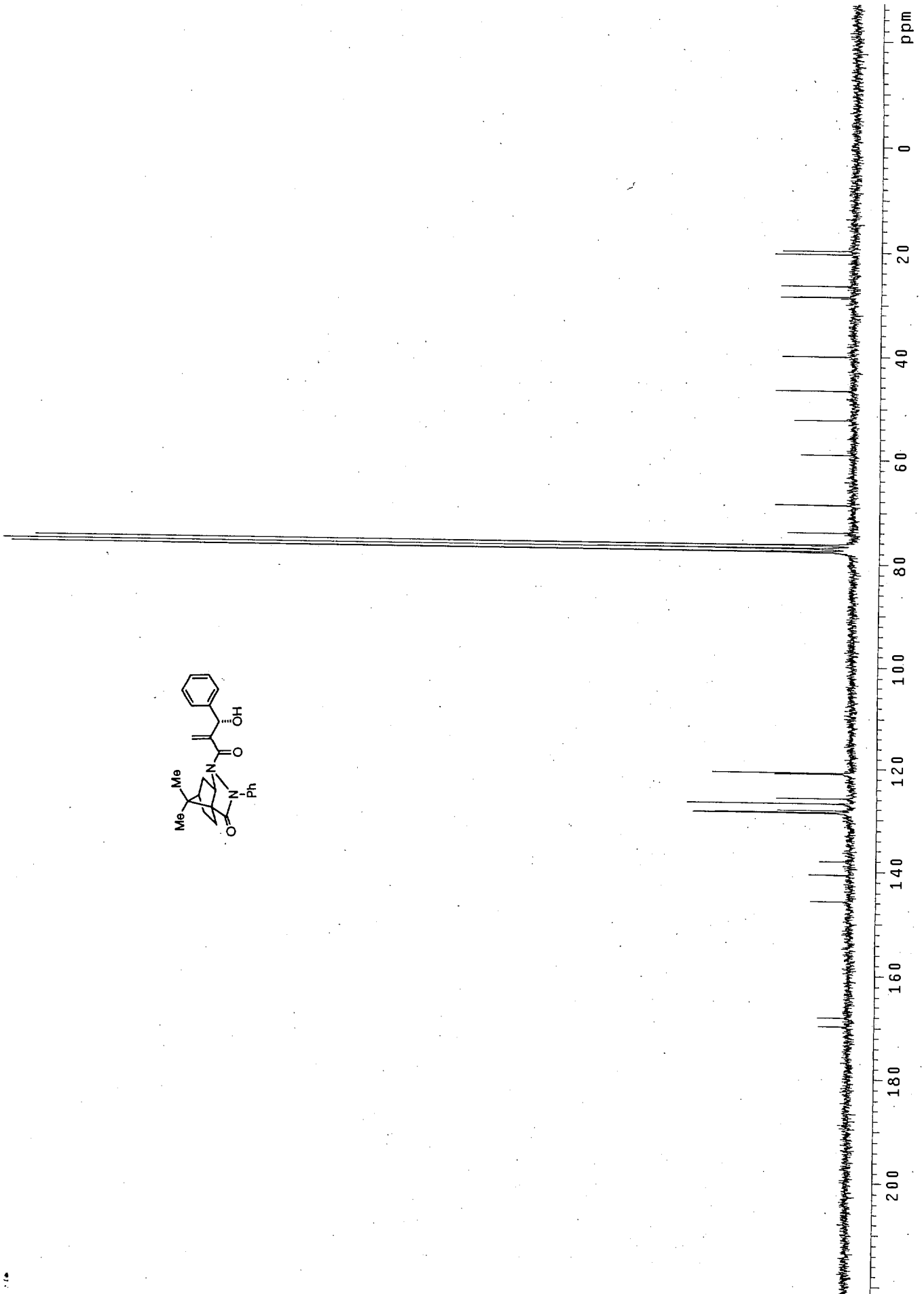
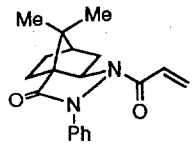


Table 1. Crystal data and structure refinement for ic6132.



Identification code	ic6132
Empirical formula	$C_{21}H_{27}N_2O_{2.50}$
Formula weight	347.45
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1$
Unit cell dimensions	a = 9.700(2) Å alpha = 90° b = 15.290(2) Å beta = 90.407(13)° c = 13.370(2) Å gamma = 90°
Volume, Z	1982.9(5) Å^3, 4
Density (calculated)	1.164 Mg/m^3
Absorption coefficient	0.076 mm^{-1}
F(000)	748
Crystal size	0.60 x 0.40 x 0.35 mm
θ range for data collection	1.52 to 27.48°
Limiting indices	$-12 \le h \le 12$, $0 \le k \le 18$, $0 \le l \le 17$
Reflections collected	4699
Independent reflections	4699 (R_{int} = 0.0000)
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4699 / 1 / 461
Goodness-of-fit on F^2	1.020
Final R indices [I>2σ(I)]	R1 = 0.0646, wR2 = 0.1899
R indices (all data)	R1 = 0.0953, wR2 = 0.2139
Absolute structure parameter	0(2)
Extinction coefficient	0.009(3)
Largest diff. peak and hole	0.814 and -0.221 eÅ^{-3}

Table 2. Bond lengths [Å] and angles [°] for 6132.

O(1)-C(1)	1.201(5)	O(2)-C(17)	1.215(6)
O(3)-C(20)	1.212(5)	O(4)-C(36)	1.217(5)
N(1)-C(1)	1.374(6)	N(1)-N(2)	1.419(5)
N(1)-C(11)	1.436(6)	N(2)-C(17)	1.356(5)
N(2)-C(3)	1.481(6)	N(3)-C(20)	1.378(6)
N(3)-N(4)	1.429(4)	N(3)-C(30)	1.437(6)
N(4)-C(36)	1.352(6)	N(4)-C(22)	1.466(5)
C(1)-C(2)	1.495(6)	C(2)-C(7)	1.514(6)
C(2)-C(3)	1.536(6)	C(2)-C(8)	1.581(6)
C(3)-C(4)	1.561(6)	C(4)-C(5)	1.534(7)
C(5)-C(8)	1.532(7)	C(5)-C(6)	1.547(8)
C(6)-C(7)	1.561(7)	C(8)-C(9)	1.506(7)
C(8)-C(10)	1.542(7)	C(11)-C(12)	1.370(6)
C(11)-C(16)	1.372(7)	C(12)-C(13)	1.396(9)
C(13)-C(14)	1.360(9)	C(14)-C(15)	1.371(9)
C(15)-C(16)	1.399(8)	C(17)-C(18)	1.488(6)
C(18)-C(19)	1.297(7)	C(20)-C(21)	1.490(6)
C(21)-C(26)	1.528(6)	C(21)-C(22)	1.547(6)
C(21)-C(27)	1.562(6)	C(22)-C(23)	1.553(6)
C(23)-C(24)	1.530(7)	C(24)-C(25)	1.539(8)
C(24)-C(27)	1.554(8)	C(25)-C(26)	1.572(8)
C(27)-C(29)	1.533(7)	C(27)-C(28)	1.536(8)
C(30)-C(35)	1.367(7)	C(30)-C(31)	1.381(8)
C(31)-C(32)	1.380(8)	C(32)-C(33)	1.314(10)
C(33)-C(34)	1.374(11)	C(34)-C(35)	1.415(10)
C(36)-C(37)	1.478(6)	C(37)-C(38)	1.307(7)
O(5)-C(41)	1.462(10)	O(5)-C(40)	1.65(2)
C(39)-C(40)	1.79(2)	C(41)-C(42)	1.420(12)

C(1)-N(1)-N(2)	111.8(3)	C(1)-N(1)-C(11)	123.5(3)
N(2)-N(1)-C(11)	118.6(3)	C(17)-N(2)-N(1)	119.0(3)
C(17)-N(2)-C(3)	129.3(3)	N(1)-N(2)-C(3)	108.0(3)
C(20)-N(3)-N(4)	111.3(3)	C(20)-N(3)-C(30)	122.6(4)
N(4)-N(3)-C(30)	119.0(3)	C(36)-N(4)-N(3)	119.0(3)
C(36)-N(4)-C(22)	130.3(3)	N(3)-N(4)-C(22)	108.1(3)
O(1)-C(1)-N(1)	124.1(4)	O(1)-C(1)-C(2)	128.2(4)
N(1)-C(1)-C(2)	107.6(3)	C(1)-C(2)-C(7)	122.3(4)
C(1)-C(2)-C(3)	104.5(3)	C(7)-C(2)-C(3)	106.3(4)
C(1)-C(2)-C(8)	115.2(4)	C(7)-C(2)-C(8)	102.9(4)
C(3)-C(2)-C(8)	103.9(3)	N(2)-C(3)-C(2)	103.1(3)
N(2)-C(3)-C(4)	120.4(3)	C(2)-C(3)-C(4)	103.6(3)
C(5)-C(4)-C(3)	100.7(4)	C(8)-C(5)-C(4)	102.7(4)
C(8)-C(5)-C(6)	103.3(4)	C(4)-C(5)-C(6)	109.1(4)
C(5)-C(6)-C(7)	103.6(4)	C(2)-C(7)-C(6)	101.2(4)
C(9)-C(8)-C(5)	115.8(4)	C(9)-C(8)-C(10)	108.4(4)
C(5)-C(8)-C(10)	114.0(5)	C(9)-C(8)-C(2)	115.3(4)
C(5)-C(8)-C(2)	91.1(3)	C(10)-C(8)-C(2)	111.6(4)
C(12)-C(11)-C(16)	120.9(5)	C(12)-C(11)-N(1)	119.1(5)
C(16)-C(11)-N(1)	119.9(4)	C(11)-C(12)-C(13)	118.6(6)
C(14)-C(13)-C(12)	121.1(5)	C(13)-C(14)-C(15)	120.1(5)
C(14)-C(15)-C(16)	119.6(6)	C(11)-C(16)-C(15)	119.6(5)
O(2)-C(17)-N(2)	122.5(4)	O(2)-C(17)-C(18)	122.5(4)
N(2)-C(17)-C(18)	114.8(4)	C(19)-C(18)-C(17)	120.9(5)
O(3)-C(20)-N(3)	123.5(4)	O(3)-C(20)-C(21)	128.7(4)
N(3)-C(20)-C(21)	107.8(3)	C(20)-C(21)-C(26)	121.9(4)
C(20)-C(21)-C(22)	103.9(3)	C(26)-C(21)-C(22)	105.9(4)
C(20)-C(21)-C(27)	115.6(4)	C(26)-C(21)-C(27)	103.4(4)
C(22)-C(21)-C(27)	104.4(3)	N(4)-C(22)-C(21)	103.3(3)
N(4)-C(22)-C(23)	120.3(4)	C(21)-C(22)-C(23)	102.6(3)

C(24)-C(23)-C(22)	102.4(4)	C(23)-C(24)-C(25)	109.0(4)
C(23)-C(24)-C(27)	101.3(4)	C(25)-C(24)-C(27)	102.5(4)
C(24)-C(25)-C(26)	104.4(4)	C(21)-C(26)-C(25)	100.4(4)
C(29)-C(27)-C(28)	106.9(4)	C(29)-C(27)-C(24)	114.2(5)
C(28)-C(27)-C(24)	114.9(4)	C(29)-C(27)-C(21)	113.6(4)
C(28)-C(27)-C(21)	115.4(4)	C(24)-C(27)-C(21)	91.6(3)
C(35)-C(30)-C(31)	120.4(5)	C(35)-C(30)-N(3)	118.8(5)
C(31)-C(30)-N(3)	120.8(4)	C(32)-C(31)-C(30)	118.9(6)
C(33)-C(32)-C(31)	122.8(7)	C(32)-C(33)-C(34)	119.0(6)
C(33)-C(34)-C(35)	121.0(6)	C(30)-C(35)-C(34)	117.9(7)
O(4)-C(36)-N(4)	122.2(4)	O(4)-C(36)-C(37)	122.5(4)
N(4)-C(36)-C(37)	115.3(4)	C(38)-C(37)-C(36)	121.2(5)
C(41)-O(5)-C(40)	103.6(7)	O(5)-C(40)-C(39)	85.0(11)
C(42)-C(41)-O(5)	107.9(7)		

Symmetry transformations used to generate equivalent atoms:

Atomic coordinates [x 10&^4&0] and equivalent isotropic displacement parameters [&GA&^2&0 x 10&^3&0] for IC6132. U(eq) is defined as one third of the trace of the orthogonalized &IU&vij&0&:&! tensor.&N

	x	y	z	U(eq)
O(1)	8778(3)	2244(2)	1632(3)	61(1)
O(2)	4467(3)	3152(3)	26(3)	74(1)
O(3)	-6240(3)	2997(2)	3416(3)	64(1)
O(4)	-10565(4)	2019(3)	4945(3)	75(1)
N(1)	6598(3)	2671(2)	1219(3)	46(1)
N(2)	5240(3)	2338(2)	1318(3)	46(1)
N(3)	-8411(3)	2562(2)	3836(3)	49(1)
N(4)	-9787(3)	2878(2)	3705(3)	46(1)
C(1)	7570(4)	2083(3)	1551(3)	47(1)
C(2)	6844(4)	1244(3)	1776(3)	45(1)
C(3)	5322(4)	1504(3)	1878(3)	46(1)
C(4)	4527(5)	679(3)	1499(4)	56(1)
C(5)	5711(5)	19(3)	1419(4)	61(1)
C(6)	6324(6)	-146(4)	2473(4)	69(1)
C(7)	7192(6)	695(3)	2686(4)	61(1)
C(8)	6836(5)	551(3)	899(4)	56(1)
C(9)	6467(6)	906(4)	-119(4)	70(1)
C(10)	8231(7)	72(5)	822(6)	83(2)
C(11)	6797(4)	3601(3)	1234(3)	48(1)
C(12)	7805(5)	3961(4)	650(4)	65(1)
C(13)	7986(6)	4867(4)	668(5)	75(2)
C(14)	7210(7)	5383(4)	1272(5)	79(2)
C(15)	6225(5)	5018(3)	1872(5)	69(1)
C(16)	6027(5)	4112(3)	1862(4)	59(1)
C(17)	4240(4)	2629(3)	689(3)	50(1)
C(18)	2826(4)	2319(3)	925(4)	57(1)
C(19)	1788(5)	2512(5)	349(5)	81(2)
C(20)	-7460(4)	3153(3)	3483(3)	47(1)
C(21)	-8206(4)	3980(3)	3242(3)	45(1)
C(22)	-9727(4)	3691(3)	3126(3)	43(1)
C(23)	-10529(5)	4513(3)	3478(4)	58(1)
C(24)	-9389(5)	5202(3)	3555(4)	61(1)
C(25)	-8778(6)	5354(4)	2511(5)	72(1)
C(26)	-7880(5)	4517(3)	2310(4)	60(1)
C(27)	-8230(5)	4678(3)	4095(4)	57(1)
C(28)	-8612(6)	4331(4)	5135(4)	73(2)
C(29)	-6871(7)	5180(5)	4215(6)	85(2)
C(30)	-8171(4)	1635(3)	3835(4)	52(1)
C(31)	-8869(5)	1095(3)	3175(4)	63(1)
C(32)	-8600(7)	209(4)	3193(5)	78(2)
C(33)	-7703(7)	-147(5)	3812(7)	89(2)
C(34)	-6984(8)	383(5)	4461(6)	97(3)
C(35)	-7220(6)	1295(5)	4487(5)	82(2)
C(36)	-10794(4)	2558(3)	4296(3)	46(1)
C(37)	-12199(4)	2874(3)	4061(4)	54(1)
C(38)	-13236(6)	2698(4)	4646(5)	77(2)
O(5)	-2007(7)	2734(4)	7530(4)	116(2)
C(39)	358(10)	2630(6)	7278(6)	112(3)
C(40)	-713(9)	3095(12)	8225(14)	235(10)
C(41)	-3227(10)	2983(6)	8101(6)	112(3)

C(42)	-4397(10)		2609(8)	7622(7)	130(3)	
O(1)	36(2)	68(2)	80(2)	-2(2)	-11(1)	-2(1)
O(2)	58(2)	85(3)	78(2)	32(2)	-15(2)	-11(2)
O(3)	40(2)	69(2)	83(2)	3(2)	6(1)	2(2)
O(4)	62(2)	81(3)	84(2)	34(2)	13(2)	15(2)
N(1)	33(2)	51(2)	53(2)	4(2)	-2(1)	-4(1)
N(2)	36(2)	46(2)	58(2)	4(2)	0(1)	-5(1)
N(3)	33(2)	50(2)	63(2)	7(2)	-1(1)	4(2)
N(4)	33(2)	47(2)	60(2)	3(2)	-4(1)	5(1)
C(1)	44(2)	54(2)	44(2)	-10(2)	-4(2)	3(2)
C(2)	43(2)	49(2)	43(2)	-4(2)	-6(2)	4(2)
C(3)	46(2)	49(2)	44(2)	-2(2)	3(2)	-3(2)
C(4)	49(2)	44(2)	74(3)	0(2)	3(2)	-7(2)
C(5)	66(3)	46(3)	72(3)	-10(2)	-1(2)	-4(2)
C(6)	79(4)	52(3)	75(3)	6(2)	-8(3)	0(3)
C(7)	70(3)	52(3)	60(3)	4(2)	-11(2)	7(2)
C(8)	55(3)	58(3)	54(2)	-14(2)	0(2)	3(2)
C(9)	75(3)	86(4)	48(2)	-21(2)	6(2)	0(3)
C(10)	69(3)	80(4)	101(4)	-24(3)	12(3)	15(3)
C(11)	38(2)	50(2)	57(2)	9(2)	-7(2)	-6(2)
C(12)	54(3)	79(4)	64(3)	4(3)	5(2)	-19(2)
C(13)	73(3)	78(4)	74(3)	27(3)	-12(3)	-30(3)
C(14)	78(4)	48(3)	112(5)	19(3)	-35(4)	-20(3)
C(15)	57(3)	50(3)	100(4)	1(3)	-3(3)	1(2)
C(16)	47(2)	56(3)	76(3)	7(2)	-1(2)	0(2)
C(17)	37(2)	57(3)	54(2)	5(2)	-5(2)	-4(2)
C(18)	40(2)	59(3)	73(3)	0(2)	0(2)	1(2)
C(19)	38(2)	102(5)	104(4)	0(4)	-12(2)	1(3)
C(20)	39(2)	52(2)	50(2)	2(2)	5(2)	-1(2)
C(21)	46(2)	45(2)	46(2)	-2(2)	2(2)	-6(2)
C(22)	40(2)	44(2)	45(2)	-3(2)	-5(2)	-1(2)
C(23)	50(2)	55(3)	68(3)	0(2)	-2(2)	7(2)
C(24)	59(3)	47(3)	77(3)	-8(2)	6(2)	-1(2)
C(25)	76(3)	48(3)	94(4)	11(3)	9(3)	-1(3)
C(26)	63(3)	55(3)	62(3)	4(2)	7(2)	-5(2)
C(27)	53(3)	61(3)	58(2)	-21(2)	-2(2)	-8(2)
C(28)	74(3)	95(4)	49(2)	-19(3)	-10(2)	-7(3)
C(29)	72(4)	82(4)	102(4)	-22(4)	-11(3)	-27(3)
C(30)	42(2)	54(3)	61(3)	18(2)	11(2)	7(2)
C(31)	51(2)	53(3)	85(3)	12(3)	3(2)	-4(2)
C(32)	69(3)	64(3)	100(4)	-2(3)	20(3)	5(3)
C(33)	70(4)	65(4)	133(6)	20(4)	29(4)	15(3)
C(34)	79(4)	97(5)	115(5)	51(5)	18(4)	46(4)
C(35)	64(3)	83(4)	98(4)	26(3)	-10(3)	19(3)
C(36)	44(2)	46(2)	50(2)	2(2)	-1(2)	-3(2)
C(37)	37(2)	59(3)	65(3)	-4(2)	-2(2)	-1(2)
C(38)	52(3)	76(4)	102(4)	5(3)	14(3)	2(3)
O(5)	140(5)	113(4)	95(3)	1(3)	33(3)	17(4)
C(39)	123(6)	110(6)	103(5)	-6(5)	-12(5)	-23(5)
C(40)	55(4)	273(18)	376(23)	195(18)	52(8)	41(7)
C(41)	141(7)	102(6)	92(5)	6(5)	15(5)	-2(5)
C(42)	117(7)	153(9)	120(7)	-27(7)	12(5)	9(7)

Table 3. Hydrogen coordinates (x 10&^4&0) and isotropic displacement parameters (&GA&^2&0 x 10&^3&0) for IC6132.&H

	x	y	z	U(eq)
H(3A)	5110(4)	1608(3)	2584(3)	56
H(4A)	3839(5)	490(3)	1975(4)	67
H(4B)	4089(5)	783(3)	855(4)	67
H(5A)	5458(5)	-518(3)	1062(4)	73
H(6A)	6902(6)	-663(4)	2479(4)	82
H(6B)	5600(6)	-216(4)	2964(4)	82
H(7A)	6907(6)	979(3)	3299(4)	73
H(7B)	8169(6)	565(3)	2723(4)	73
H(9A)	7234(6)	1228(4)	-380(4)	105
H(9B)	5684(6)	1288(4)	-64(4)	105
H(9C)	6245(6)	431(4)	-561(4)	105
H(10A)	8483(7)	-159(5)	1466(6)	125
H(10B)	8926(7)	475(5)	605(6)	125
H(10C)	8153(7)	-398(5)	349(6)	125
H(12A)	8356(5)	3609(4)	250(4)	79
H(13A)	8648(6)	5121(4)	261(5)	90
H(14A)	7348(7)	5985(4)	1277(5)	95
H(15A)	5692(5)	5371(3)	2283(5)	83
H(16A)	5377(5)	3857(3)	2278(4)	71
H(18A)	2683(4)	1982(3)	1495(4)	69
H(19A)	1923(5)	2848(5)	-222(5)	98
H(19B)	910(5)	2313(5)	506(5)	98
H(22A)	-9937(4)	3571(3)	2421(3)	52
H(23A)	-11229(5)	4682(3)	2994(4)	69
H(23B)	-10960(5)	4415(3)	4121(4)	69
H(24A)	-9663(5)	5739(3)	3902(4)	73
H(25A)	-8213(6)	5877(4)	2502(5)	87
H(25B)	-9502(6)	5412(4)	2011(5)	87
H(26A)	-8167(5)	4219(3)	1703(4)	72
H(26B)	-6907(5)	4657(3)	2271(4)	72
H(28A)	-9462(6)	4011(4)	5091(4)	109
H(28B)	-8718(6)	4813(4)	5588(4)	109
H(28C)	-7894(6)	3951(4)	5375(4)	109
H(29A)	-6596(7)	5408(5)	3578(6)	128
H(29B)	-6170(7)	4792(5)	4464(6)	128
H(29C)	-6994(7)	5653(5)	4677(6)	128
H(31A)	-9509(5)	1326(3)	2726(4)	76
H(32A)	-9075(7)	-152(4)	2749(5)	93
H(33A)	-7557(7)	-748(5)	3810(7)	107
H(34A)	-6332(8)	137(5)	4891(6)	116
H(35A)	-6743(6)	1653(5)	4933(5)	98
H(37A)	-12348(4)	3205(3)	3486(4)	64
H(38A)	-13097(6)	2368(4)	5222(5)	92
H(38B)	-14113(6)	2902(4)	4486(5)	92
H(39A)	1309(10)	2725(6)	7449(6)	169
H(39B)	156(10)	2902(6)	6647(6)	169
H(39C)	182(10)	2013(6)	7231(6)	169
H(40A)	-631(9)	2817(12)	8874(14)	282

H(40B)	-658(9)	3727(12)	8277(14)	282
H(41A)	-3149(10)	2769(6)	8782(6)	134
H(41B)	-3314(10)	3615(6)	8121(6)	134
H(42A)	-5214(10)	2763(8)	7983(7)	195
H(42B)	-4303(10)	1984(8)	7608(7)	195
H(42C)	-4467(10)	2827(8)	6950(7)	195

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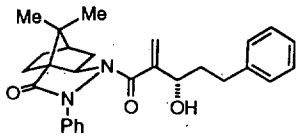
Space Group and Cell Dimensions Monoclinic, P 21
a 11.387(3) b 9.024(6) c 11.8731(24)
beta 98.661(20)
Volume 1206.2(9)A**3



Empirical formula : C28 H32 N2 O3

Cell dimensions were obtained from 25 reflections with 2Theta angle in the range 19.40 - 28.02 degrees.

Crystal dimensions : 0.50 X 0.30 X 0.12 mm

FW = 444.57 Z = 2 F(000) = 475.93

Dcalc 1.224Mg.m-3, mu 0.07mm-1, lambda 0.70930A, 2Theta(max) 51.8

The intensity data were collected on a Nonius diffractometer, using the theta/2theta scan mode.
The h,k,l ranges are :-- -14 13, 0 11, 0 14
No. of reflections measured 2644
No. of unique reflections 2522
No. of reflections with Inet > 2.0sigma(Inet) 1574
Absorption corrections were made.
The minimum and maximum transmission factors are 0.828540 and 0.999632.

The last least squares cycle was calculated with
65 atoms, 298 parameters and 1574 out of 2522 reflections.
Weights based on counting-statistics were used.

The residuals are as follows :--
For significant reflections, RF 0.050, Rw 0.036 GoF 3.07
For all reflections, RF 0.093, Rw 0.037.
where RF = Sum(Fo-Fc)/Sum(Fo),
Rw = Sqrt[Sum(w(Fo-Fc)**2)/Sum(wFo**2)] and
GoF = Sqrt[Sum(w(Fo-Fc)**2)/(No. of reflns - No. of params.)]
The maximum shift/sigma ratio was 0.000.

In the last D-map, the deepest hole was -0.210e/A**3,
and the highest peak 0.180e/A**3.

Secondary ext. coeff. = 0.003258 sigma = 0.003736

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The following Atoms are from the CD File

* Indicates that there are Symmetry Equivalents of an atom.

Name	x	y	z
O(1)	0.96525	0.51916	0.13440
O(2)	1.03740	0.07769	0.09704
O(3)	1.05120	0.87900	0.44052
N(1)	1.04980	0.52685	0.32014
N(2)	1.00315	0.67488	0.32845
C(1)	1.01956	0.45948	0.21698
C(2)	1.04865	0.29375	0.21582
C(3)	1.03951	0.21211	0.30575
C(4)	1.06847	0.23402	0.10005
C(5)	1.19466	0.25178	0.07771
C(6)	1.28678	0.15725	0.15261
C(7)	1.07854	0.75743	0.40816
C(8)	1.19045	0.67255	0.43904
C(9)	1.15476	0.51026	0.40871
C(10)	1.27018	0.44414	0.37647
C(11)	1.35945	0.56809	0.41264
C(12)	1.37351	0.58931	0.54280
C(13)	1.25524	0.67179	0.56035
C(14)	1.28925	0.70757	0.36650
C(15)	1.35277	0.85877	0.40067
C(16)	1.25102	0.71384	0.23654
C(1A)	1.40934	0.17276	0.12338
C(2A)	1.49300	0.26283	0.18485
C(3A)	1.60472	0.27654	0.15425
C(4A)	1.63703	0.20134	0.06447
C(5A)	1.55405	0.11493	0.00327
C(6A)	1.44236	0.09958	0.03114
C(1B)	0.87810	0.69988	0.30306
C(2B)	0.83708	0.81923	0.23771
C(3B)	0.71747	0.84551	0.21726
C(4B)	0.63966	0.74939	0.25924
C(5B)	0.68248	0.63166	0.32511
C(6B)	0.80159	0.60652	0.34837
HO(2)	0.95124	0.09467	0.06782
H(3)	1.02509	0.25717	0.37810
H(3')	1.04719	0.09911	0.30529
H(4)	1.01350	0.29589	0.03685
H(5)	1.19845	0.22226	-0.00889
H(5')	1.22144	0.36535	0.09322
H(6)	1.25888	0.03908	0.14274
H(6')	1.28578	0.18451	0.24250
H(9)	1.13054	0.45183	0.48422
H(10)	1.29486	0.33830	0.42290
H(10')	1.26092	0.41754	0.28609
H(11)	1.44404	0.55530	0.38189
H(12)	1.45178	0.65885	0.57693
H(12')	1.38459	0.48504	0.59070
H(13)	1.27214	0.78080	0.59611
H(13')	1.20777	0.60760	0.61856
H(15)	1.28395	0.94180	0.38677
H(15')	1.42093	0.88078	0.34906

H(16")	1.20989	0.60906	0.20662
H(2A)	1.47269	0.31823	0.24897
H(3A)	1.66475	0.33967	0.20557
H(4A)	1.71795	0.20989	0.03887
H(5A)	1.57762	0.05537	-0.05957
H(6A)	1.38565	0.02834	-0.01493
H(2B)	0.89380	0.88774	0.20710
H(3B)	0.68548	0.92978	0.16967
H(4B)	0.55459	0.76730	0.24027
H(5B)	0.62588	0.56292	0.36015
H(6B)	0.83974	0.52502	0.40494

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O(1)-C(1)	1.205(8)	C(12)-H(12)	1.115(6)
O(2)-C(4)	1.454(9)	C(12)-H(12')	1.097(8)
O(2)-HO(2)	1.002(4)	C(13)-H(13)	1.077(7)
O(3)-C(7)	1.218(7)	C(13)-H(13')	1.104(6)
N(1)-N(2)	1.446(8)	C(14)-C(15)	1.569(10)
N(1)-C(1)	1.364(8)	C(14)-C(16)	1.540(9)
N(1)-C(9)	1.476(7)	C(15)-H(15)	1.079(7)
N(2)-C(7)	1.394(8)	C(15)-H(15')	1.077(6)
N(2)-C(1B)	1.428(7)	C(15)-H(15")	1.082(7)
C(1)-C(2)	1.532(11)	C(16)-H(16)	1.076(6)
C(2)-C(3)	1.314(10)	C(16)-H(16')	1.100(7)
C(2)-C(4)	1.525(9)	C(16)-H(16")	1.091(7)
C(3)-H(3)	0.986(6)	C(1A)-C(2A)	1.375(14)
C(3)-H(3')	1.024(7)	C(1A)-C(6A)	1.379(11)
C(4)-C(5)	1.509(10)	C(2A)-C(3A)	1.380(14)
C(4)-H(4)	1.061(7)	C(2A)-H(2A)	0.967(8)
C(5)-C(6)	1.529(10)	C(3A)-C(4A)	1.360(14)
C(5)-H(5)	1.069(6)	C(3A)-H(3A)	1.019(8)
C(5)-H(5')	1.077(7)	C(4A)-C(5A)	1.350(15)
C(6)-C(1A)	1.495(11)	C(4A)-H(4A)	1.016(8)
C(6)-H(6)	1.114(8)	C(5A)-C(6A)	1.369(13)
C(6)-H(6')	1.097(6)	C(5A)-H(5A)	0.989(8)
C(7)-C(8)	1.485(8)	C(6A)-H(6A)	1.011(8)
C(8)-C(9)	1.548(9)	C(1B)-C(2B)	1.368(10)
C(8)-C(13)	1.516(7)	C(1B)-C(6B)	1.378(9)
C(8)-C(14)	1.549(8)	C(2B)-C(3B)	1.368(10)
C(9)-C(10)	1.543(8)	C(2B)-H(2B)	1.001(7)
C(9)-H(9)	1.110(5)	C(3B)-C(4B)	1.385(14)
C(10)-C(11)	1.529(10)	C(3B)-H(3B)	0.984(8)
C(10)-H(10)	1.117(7)	C(4B)-C(5B)	1.365(13)
C(10)-H(10')	1.089(6)	C(4B)-H(4B)	0.974(7)
C(11)-C(12)	1.541(9)	C(5B)-C(6B)	1.362(9)
C(11)-C(14)	1.546(10)	C(5B)-H(5B)	1.027(7)
C(11)-H(11)	1.087(5)	C(6B)-H(6B)	1.045(7)
C(12)-C(13)	1.580(9)		

C(4)-O(2)-HO(2)	94.7(5)	C(13)-C(12)-H(12)	109.7(6)
N(2)-N(1)-C(1)	115.3(5)	C(13)-C(12)-H(12')	111.7(5)
N(2)-N(1)-C(9)	108.1(5)	H(12)-C(12)-H(12')	105.7(5)
C(1)-N(1)-C(9)	131.5(5)	C(8)-C(13)-C(12)	100.3(4)
N(1)-N(2)-C(7)	110.2(5)	C(8)-C(13)-H(13)	113.7(6)
N(1)-N(2)-C(1B)	119.8(5)	C(8)-C(13)-H(13')	112.5(5)
C(7)-N(2)-C(1B)	123.5(5)	C(12)-C(13)-H(13)	112.2(5)
O(1)-C(1)-N(1)	124.1(7)	C(12)-C(13)-H(13')	110.1(6)
O(1)-C(1)-C(2)	121.0(6)	H(13)-C(13)-H(13')	107.9(5)
N(1)-C(1)-C(2)	114.7(5)	C(8)-C(14)-C(11)	91.0(5)
C(1)-C(2)-C(3)	119.8(6)	C(8)-C(14)-C(15)	112.3(5)
C(1)-C(2)-C(4)	114.5(6)	C(8)-C(14)-C(16)	116.4(5)
C(3)-C(2)-C(4)	125.1(7)	C(11)-C(14)-C(15)	115.0(5)
C(2)-C(3)-H(3)	121.4(7)	C(11)-C(14)-C(16)	116.0(6)
C(2)-C(3)-H(3')	122.5(6)	C(15)-C(14)-C(16)	106.1(6)
H(3)-C(3)-H(3')	116.2(7)	C(14)-C(15)-H(15)	105.6(5)
O(2)-C(4)-C(2)	107.3(5)	C(14)-C(15)-H(15')	110.8(6)